



SDI Review Form 1.6

Journal Name:	International Research Journal of Pure and Applied Chemistry
Manuscript Number:	2013_IRJPAC_7876
Title of the Manuscript:	A theoretical study of the relationships between electronic structure and anti-inflammatory and anti-cancer activities of a series of 6,7-substituted-5,8-quinolinequinones
Type of the Article	research

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:

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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)
Compulsory REVISION comments	This manuscript describes the search of quantum-chemical model-based relationships between electronic structure and anti-inflammatory and antiproliferative activity against HL60 and T-cells of a group of 6,7-substituted-5,8-quinolinequinones. I recommend this paper for publishing in International Research Journal of Pure and Applied Chemistry after some corrections. I have the following question/comments to the authors. General remarks:	As the phrase "The part dedicated to opiates and cannabinoids is useless" we removed it. But this removal demanded that the ensuing phrases be rewritten. Therefore we have proceeded to rewrite part of the Introduction section. We have downloaded, analyzed and included several new references. We also downloaded and analyzed all the references suggested by the referee. Thanks to the referee for mentioning the work by Fischer & Renouf (Fischer O, Renouf E, Ueber einige Abkömmlinge des Orthooxychinolins, Ber. Deut. Chem. Ges., 1884;17:1642-1646). We included it and also we mentioned and cited Lavendamycin (Thanks again). Most of the remaining references suggested by the referee are not pertinent to the article; therefore we did not include them. DISCUSSION SECTION. The referee asked us "to strengthening presented conclusions by experimental results from other papers". Unhappily we cannot do this for the following reasons: 1. These molecules were synthesized only recently. All experimental data known about them is in Mulchin's paper. There are no other experimental results. We have searched again to find if a new paper appeared during last months



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	<u>The Intruduction part:</u> The part dedicated to opiates and cannabinoids is useless. The most important representative of 5,8-quinolinequinones are: streptonigrin or lavendamycin. They both possess quinoline-5,8-dione subunit. The idea to find relationships between the electronic structure and the biological activities of 6,7-substituted-5,8-quinolinequinones is good target for the research. It will be nice to present in introduction part the present knowledge about quinoline-5,8-dione derivatives. To show how other authors correlate the theoretical studies with their reactivity. Please reconsider the structure of 5,8-dihydro-5,8-dioxoquinoline as a	but we found nothing. 2. The method used here belongs to the class of formal models. Then, the only way to make acceptable comparisons with other studies is that they employ similar ways of working. Anyway there are no other results in the literature. On the other hand, if we employ this method to study several families of molecules with biological activities measured with the same method we shall be in position to make possible generalizations. As far as we know, the only systems in which this kind of knowledge accumulation is occurring is for the case of cannabinoid receptors ligands. We expect that the referee will be satisfied with the changes made to the paper. Thanks.
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	reference molecule see e.g. Australian Journal of Chemistry, 1982, 35, 1439 – 1450. Next recommended other see e.g. Tetrahedron, 2011, 67, 1763 – 1767 J. Mol. Struct. 2011, 986, 39 – 48. Organic and Biomolecular Chemistry, 2012, 10, 6375 – 638 Eur. J. Inorg. Chem. 2011, 2413 – 2421. Chemische Berichte, 1884, 17, 1645 Phosphorus Sulfur Silicon, Relat. Elem. 2012, 187, 564 – 572. Journal of the American Chemical Society, 1955, 77, 37 – 39 Journal of Organic Chemistry, 1985, 50, 5782 – 5789	
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	Bioorg. Med. Chem. 2011, 19, 1606 – 12. Journal of Organic Chemistry, 1985, 50, 5782 - 5789 Journal of Organic Chemistry, 1985, 50, 4276 – 4281 Journal of Medicinal Chemistry, 1986 , 29, 1329 – 1340 4. DISCUSSION This part is much, much better. Personally I suggest to strengthening presented conclusions by experimental results from other papers (see comments to Introduction).	
<u>Minor</u> REVISION comments		
<u>Optional/General</u> comments		