



SDI Review Form 1.6

Journal Name:	Asian Journal of Chemical Sciences
Manuscript Number:	Ms_AJOCS_40462
Title of the Manuscript:	Comparison of 6-311G(d) and 3-21G(DFT/HF) Methods of 3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one
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:

(<http://www.sciencedomain.org/page.php?id=sdi-general-editorial-policy#Peer-Review-Guideline>)

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	<p>1. Page 1, Line 17-18. As reads: "In fact, some studies are more accurate and reliable results than the experimental method." This is an untrue statement – computational studies are designed to provide a comparison to experimentally determined physical properties, thermodynamic and kinetic data. Refinement of computational methods is driven by a desire to achieve consistency and agreement with experimental results, not the other way around. There is no substitute for experimentation in the determination of molecular structure and QSAR.</p> <p>2. The authors provide a great deal of data in Tables 1-11 and Figures 1-5, but offer no discussion of the results for these computationally determined values. What is the purpose of using multiple methods? A comparison of these methods may be informative to the reader provided the authors compare and contrast the results obtained from the different levels of theoretical computations with experimentally determined values. In my opinion, this work must include a much more thorough discussion to give context for the reader.</p>	
Minor REVISION comments	<p>1. Page 1, lines 16-17. Awkward sentence structure. As reads: "Many properties of molecules with theoretical calculation methods can be calculated without having to experiment." Recommend changing to read: "Many properties of molecules may be theoretically calculated without the need to experimentally determine them."</p> <p>2. Page 3, Line 100. Omit the words, "and chemical".</p> <p>3. Figure 2 is of insufficient resolution and appears compressed. It should be redrawn to correct these issues to improve readability.</p>	
Optional/General comments		

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