



SDI Review Form 1.6

Journal Name:	Physical Science International Journal
Manuscript Number:	Ms_PSIJ_46207
Title of the Manuscript:	DFT-QSAR and Molecular Docking Studies on 1,2,3-Triazole-Dithiocarbamate Hybrids as Potential Anticancer Agents
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	<ul style="list-style-type: none"> Using electronic descriptors to determine structure activity relationship is an interesting work, but the number of compounds is not enough to build a strong model that author can use it to predict new compounds. The equation of obtained model contains six descriptors while authors used only eight compounds which explain the high value of R2. What was done for inspection the quality of pdb file? Usually RMSD value is used to validate docking protocol, which means that a root mean square deviation value is necessary step in molecular docking process, authors did not mentioned it. The interactions obtained in molecular docking don't explain the high activity of compound "D" and low activity of compound "C"(it shows similar interactions). 	All necessary correction have been made.
Minor REVISION comments		
Optional/General comments		

PART 2:

	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)
Are there ethical issues in this manuscript?	(If yes, Kindly please write down the ethical issues here in details)	