



SDI Review Form 1.6

Journal Name:	International Research Journal of Pure and Applied Chemistry
Manuscript Number:	Ms_IRJPAC_37402
Title of the Manuscript:	COMPUTATIONAL CHEMISTRY STUDIES ON THE ADSORPTION/CORROSION INHIBITIVE POTENTIAL OF 2-(2-heptadecyl-4,5-dihydro-1H-imidazol-1-yl) ethan-1-ol)
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		
Minor REVISION comments	<p>The work presents a scientific interest confirmed by the study of corrosion inhibition of the iron surface by the adsorption process. The authors used the adequate molecular modeling tools to demonstrate this corrosion inhibition. Through their sufficient and relevant results, it's also important to point out that the interpretations and the conclusion are justified by the calculation data and are consistent with the objectives assigned for their work. However, I would have liked to see a consolidation of the corrosion inhibition results through an experimental cyclic voltammetry study, this last remarque is in no way diminishes the quality of this scientific work.</p> <p>The paper has been written adequately. However, the following remarks should be taken into consideration :</p> <p>1-No other metal is available to replace iron in all its many applications (line 25-26). Reformulate this sentence since there are many composite materials that have properties and applications better than iron. (Nanomaterials-based composite)</p> <p>2-It is necessary to add other determining parameters during the adsorption of the amine-nitrogen compounds on the iron surface (line 33-34)</p> <p>3-The author must put the expression that calculates the adsorbate-adsorbent interaction energy during the absorption process (line 190 see also table 1).</p> <p>4-Add the nature of physical or chemical adsorption in the conclusion and abstract.</p> <p>5-The formulas (equations: 5 to 9) must be written by an equation editor</p>	<p>Thank you for your remarks. I agree with number 1,2 and 5 remarks and I have made the necessary corrections and they are highlighted in the manuscript. The number 3 remark is the first equation in chapter 2 (Computational details). For the number 4 remark, it is stated that the molecule is physically adsorbed on the iron surface, which is physical adsorption (Physisorption).</p>
Optional/General comments	Update references: Ref 28 and Ref 14 to18	No comment.