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The Editor-in Chief,
Journal of Applied Surfaces and Interfaces.

Sir,

SUBMISSION COVER LETTER

On behalf of the authors, I present to you the manuscript of our original work titled '***Density Functional Theory and Molecular Dynamic Simulation Studies on the Corrosion Inhibition of Some Thiosemicarbazide Derivatives on Aluminium Metal***' which we all matually agree to submit for publication with the ***Journal of Applied Surfaces and Interfaces (JASI)***. This manuscript has not been published, or is not under consideration for publication elsewhere.
From the findings presented in this work:

1. The results obtained theoretically were in good agreement with that reported experimentally by Fouda *et al*., (1986).
2. It was also established from the adsorption or binding energy of the thiosemicarbazides molecules on the Al surface to be relatively low signifying the mechanism of physical adsorption and therefore serving as weak inhibitors on Al surface.
3. The reference thiosemicarbazide molecule was found to have the least inhibition efficiency in terms of adsorption or binding energies relative to the other five derivatives which are more promising to serve as corrosion inhibitors on Al surface.
4. The thiosemicarbazide derivative established to have the highest adsorption or binding energy and therefore a better Al corrosion inhibitor is relatively large in size with additional functional groups including C=O and C=S absent in others.

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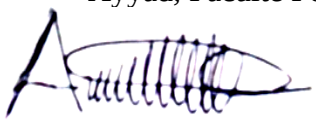

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