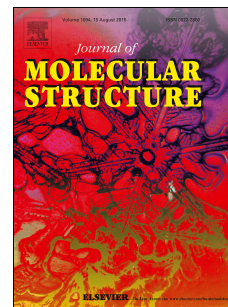


# Accepted Manuscript

Synthesis, crystal structure, DFT, molecular dynamics simulation and evaluation of the anticorrosion performance of a new pyrazolotriazole derivative

Youness El Bakri, Lei Guo, El Hassane Anouar, Abdallah Harmaoui, Abdelkader Ben Ali, El Mokhtar Essassi, Joel T. Mague



PII: S0022-2860(18)31056-1

DOI: [10.1016/j.molstruc.2018.08.107](https://doi.org/10.1016/j.molstruc.2018.08.107)

Reference: MOLSTR 25628

To appear in: *Journal of Molecular Structure*

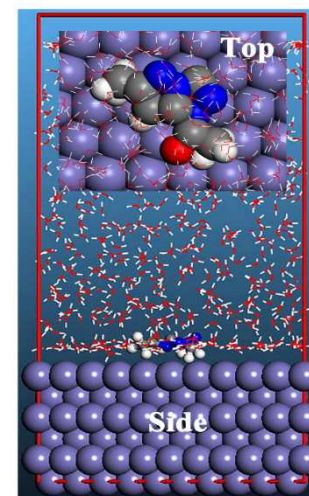
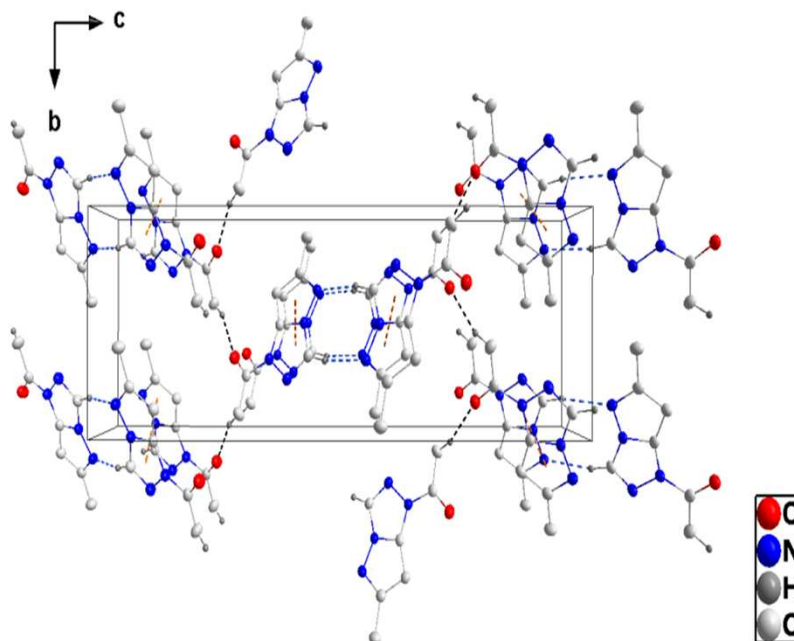
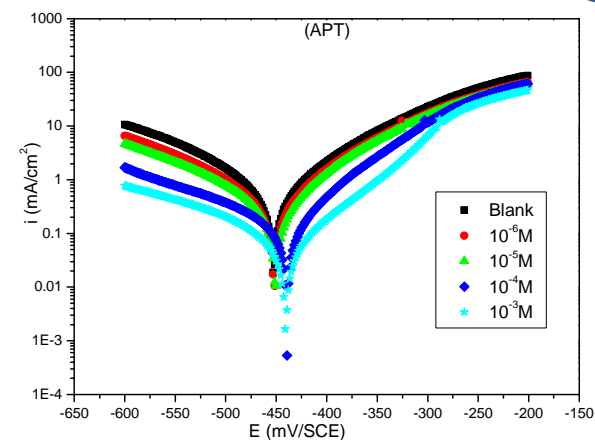
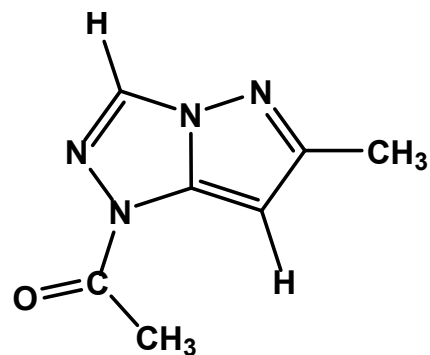
Received Date: 29 July 2018

Revised Date: 30 August 2018

Accepted Date: 31 August 2018

Please cite this article as: Y. El Bakri, L. Guo, E.H. Anouar, A. Harmaoui, A. Ben Ali, E.M. Essassi, J.T. Mague, Synthesis, crystal structure, DFT, molecular dynamics simulation and evaluation of the anticorrosion performance of a new pyrazolotriazole derivative, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.08.107.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



**2D structure (up right), molecular packing (bottom right), Polarization curves for carbon steel in the absence (blank) and presence of APT at different concentrations (up left) and MD simulation of APT on Fe surface (bottom left).**

Download English Version:

<https://daneshyari.com/en/article/10135053>

Download Persian Version:

<https://daneshyari.com/article/10135053>

[Daneshyari.com](https://daneshyari.com)