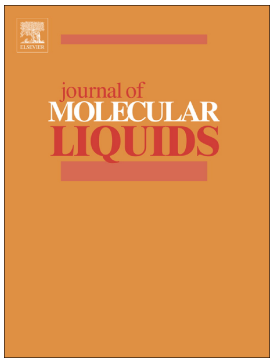

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Piperine derivatives as green corrosion inhibitors on iron surface; DFT, Monte Carlo dynamics study and complexation modes

M. E. Belghiti[1,*], S. Echihi[2,3], A. Mahsoune[4], Y. Karzazi[1], A. Aboulmouhajir[4,5], A. Dafali[1], I. Bahadur[6,*]

[1]Laboratory of Applied Analytical Chemistry, Materials and Environment (URAC 18), Faculty of Sciences, University Mohammed Premier, B.P. 4808, 60046 Oujda, Morocco.
[2]Laboratory of Water and Environment, Faculté des Sciences, Université Chouaib Doukkali, BP20, 24000 El Jadida, Morocco
[3]Laboratory of Materials, Nanotechnology and Environment, Faculty of Science, University Mohamed-V, Av. IbnBattouta, BP 1014 Agdal-Rabat, Morocco
[4]Equipe of Molecualr Modelling and Spectroscopy, Sciences Faculty, University of Chouai Doukkali, Morocco
[5]Organic synthesis, Extraction and Valorization laboratory, Equipe of Extraction Spectroscopy and Valorization, Sciences Faculty of Ain Chock, University of Hassan II, Morocco
[6]Department of Chemistry, School of Mathematical and Physical Sciences, Materials Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural, Sciences, North-West University (Mafikeng Campus), Private Bag X2046, Mmabatho 2735, South Africa

[*]Corresponding authors: bahadur.indra@nwu.ac.za; elbelghiti10@gmail.com

ABSTRACT

In the present paper, the interaction of three Piperine derivatives namely: 5-(1,3-benzodioxol-5-yl)-1-(piperidin-1-yl) pent-2-en-1-one (S_1), 5-(1,3-benzodioxol-5-yl)-1-(piperidin-1-yl) penta-2,4-dien-1-one (S_2) and 5-(1,3-benzodioxol-5-yl) penta-2,4-dienoic acid (S_3) with iron (Fe) have been investigated theoretically by means of DFT method at the B_3LYP/LANL2DZ high basis set. The interaction with iron surface therefore all possible Fe-inhibitor interaction modes at —O— and >N— active sites. The preferred complexes are those in which the Fe-atoms is in mono-dentate mode to the studied inhibitors. The quantum chemical properties most relevant to their potential action as corrosion inhibitors have also been calculated in both isolated and Fe-inhibitor (S_i) complex form for comparison. The values of the calculated interaction energy are consistent with the experimentally observed highest corrosion inhibition efficiency trend for the three S_1FeN_{26}, S_2FeN_{24} & S_3FeO_{26} complexes. The chemical reactivity and site selectivity of the molecule has been determined with the help of global and local reactivity descriptors of Fe-inhibitor (S_i) complexes. The calculations show that