



# Experimental and theoretical examinations of triazole linked saccharin derivatives as organic corrosion inhibitors for mild steel in hydrochloric acid

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## ABSTRACT

The new triazole linked saccharin derivatives namely, 2-(3-methyl-1H-1,2,4-triazol-5-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide (MTD) and 2-(3-isopropyl-1H-1,2,4-triazol-5-yl)benzo[d]isothiazol-3(2H)-one 1,1-dioxide (ITD) were synthesized under microwave irradiation method. The newly synthesized inhibitors were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, FT-IR and mass spectroscopic techniques. The ability for these two compounds to act as corrosion inhibitors for mild steel (MS) in 0.5 M HCl was confirmed by electrochemical impedance spectroscopy (EIS), weight loss and potentiodynamic polarization studies. Within the scope of concentrations and temperatures studied, the tested MTD and ITD demonstrated significant anticorrosion performances, with highs of 94 and 96% at 0.8 mM, respectively. Polarization studies revealed that the MTD and ITD behave as mixed-type inhibitors. The examined inhibitors strong adsorption mirrored the Langmuir model with excellent correlation values. The values obtained of the standard adsorption free energy indicated the typical physisorption and chemisorption behaviour of MTD and ITD on MS. Further, SEM, XPS and XRD were used to analyze the surface morphology of the MS surface. DFT calculations was employed as a supplementary tool to demonstrate the reported inhibition efficiencies.

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## 1. Introduction

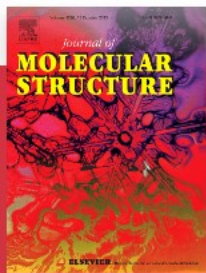
Metallic materials are affected by the outcome of their contact with the corrosive media that surrounds them during storage, service, or transport; this is known as metallic corrosion. Metal corrosion causes enormous economic loss and resource waste [1]. It also leads to significant vulnerabilities and poses possible dangers to the environment and human life [2]. As a result, corrosion shielding for metallic materials is now a rich area for researchers. Excellent physicochemical and mechanical properties fa-

vor the utility of MS as a demanding construction, manufacturing material and many other applications. However, it has poor corrosion resistance, particularly in acidic circumstances, resulting in significant financial and industrial losses [3]. The use of corrosion inhibitors is an efficient approach to prevent mild steel from corroding. In general, organic inhibitors are often utilized in a wide range of conditions, primarily in an acidic environment [4]. The growth of a protective barrier upon that metal surface via the chemisorption or physisorption process is primarily responsible for these organic inhibitor's corrosion inhibition efficacy [5].

During the past decade, a number of corrosion inhibitors have been reported. The majority of effective corrosion inhibitors are heterocyclic compounds. The Heterocyclic corrosion inhibitors contain a host of functional groups with strong electronegativity [6].

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