**ABSTRACT**

The inhibition efficiency (IE) of thiazolo thiadiazole (TT) derivatives on the mild steel corrosion in 1 M sulphuric acid was studied by weight-loss and electrochemical studies. The outcomes attained from these studies showed that the efficiency of the inhibitors was found to increase with increasing inhibitor concentration. Theoretical fitting of Langmuir isotherms were tried to elucidate the adsorption mode. Potentiodynamic Polarization studies revealed that these thiazolo thiadiazole derivatives performed as mixed type. DFT calculations have been performed to study the adsorption sites of these compounds taking part in the inhibition process through acceptor-donor interaction. Negative values of the interaction energy and high values of the binding energy obtained by molecular simulations (MC and MD) show that the synthesized thiazolo thiadiazolemolecules are strongly adsorbed on the iron surface with maximum protection against corrosion.