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Supplementary Materials

Investigating Quinazolinone Derivatives as Corrosion Inhibitors for Mild Steel in 1.0 M HCl: Experimental Insights, DFT Calculations, and MC Simulations

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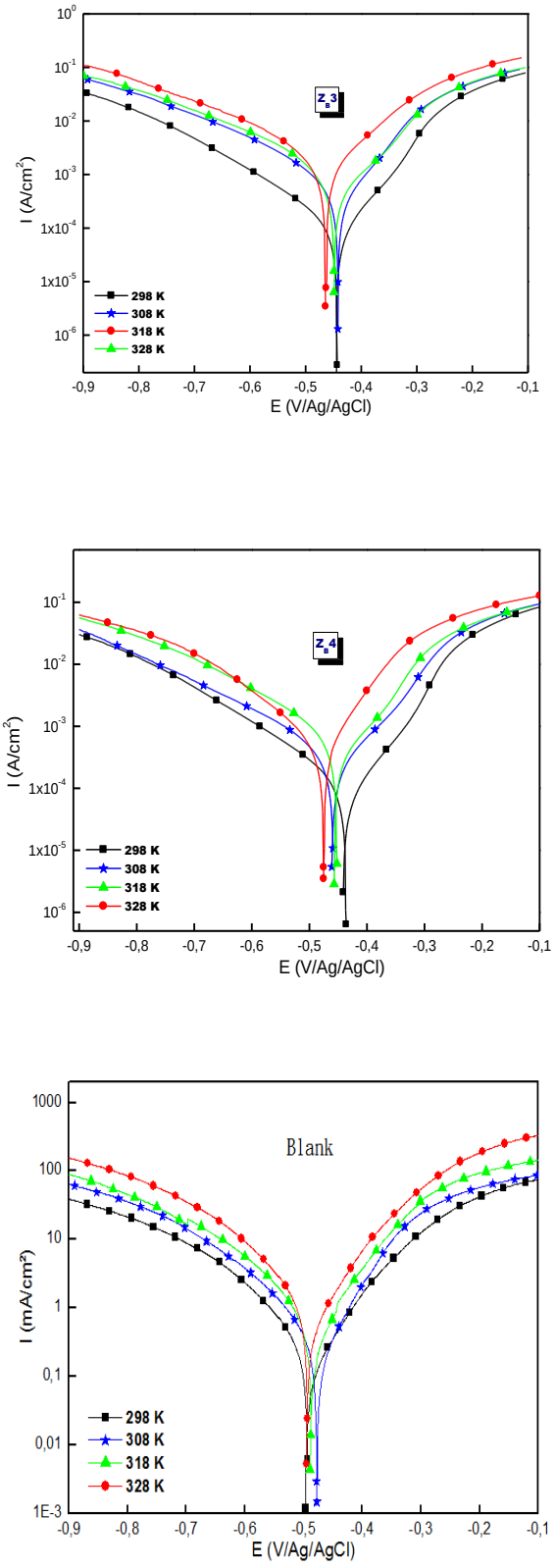


Figure S1. M-steel's polarization curves in 1 M HCl in the presence and absence of inhibitors at various temperatures

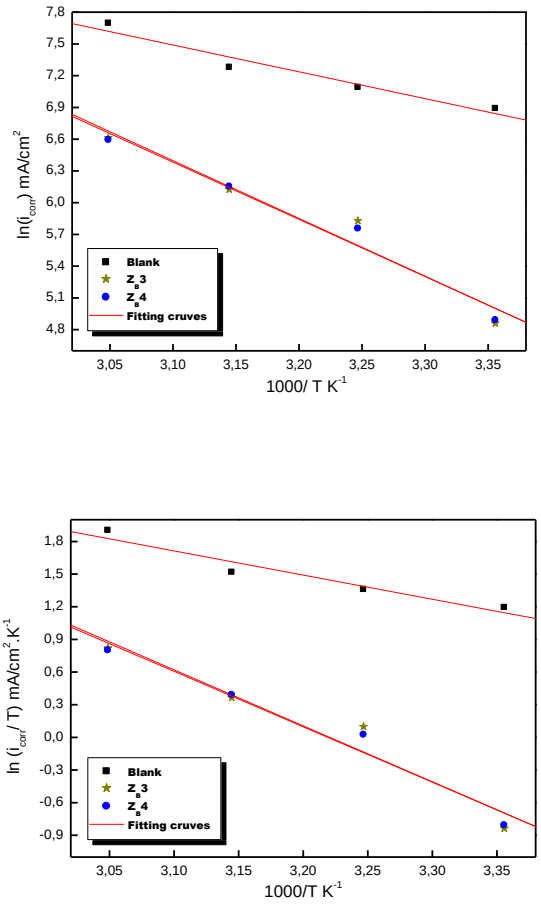


Figure S2. Straights recompild of ln (i_{corr} /T) vs the opposit of the temperature employed to collect the activation parameters of ZB3 & ZB4

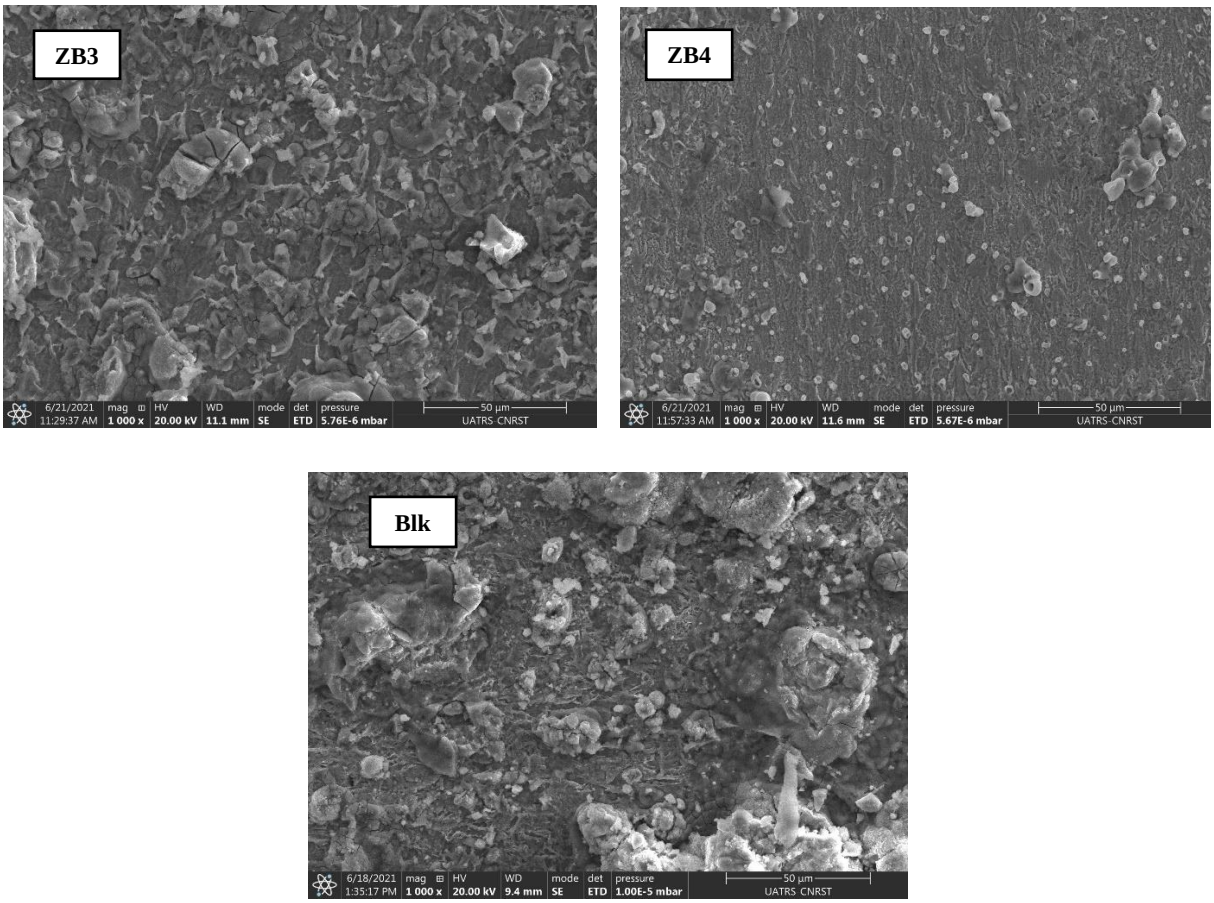


Figure S3. SEM micrographs of the steel after 6H immersion in 1M HCL before and after addition of ZB3 and ZB4

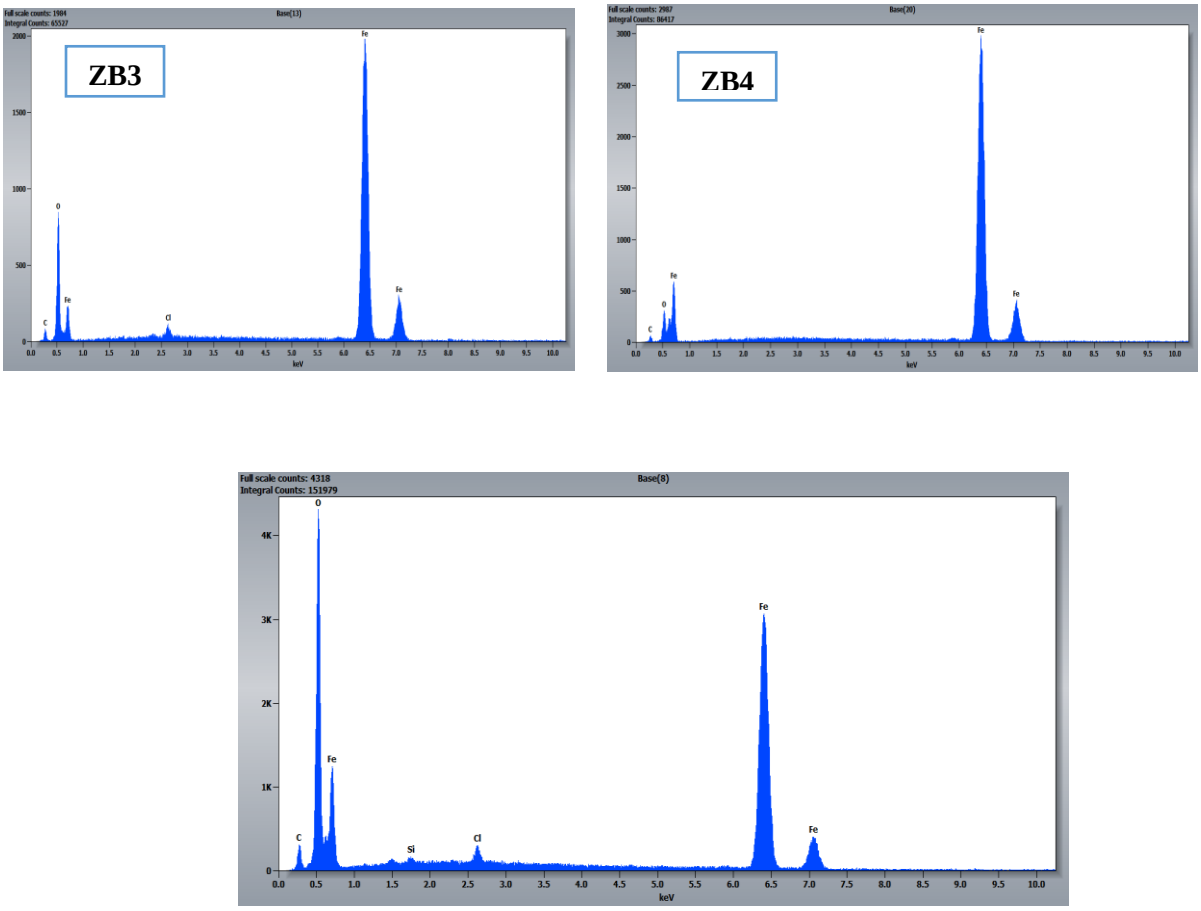


Figure S4. EDS spectra of mild steel submerged in 1.0 M HCl despite any study molecules (blank) and with 10^{-3} M of ZB3 and ZB4

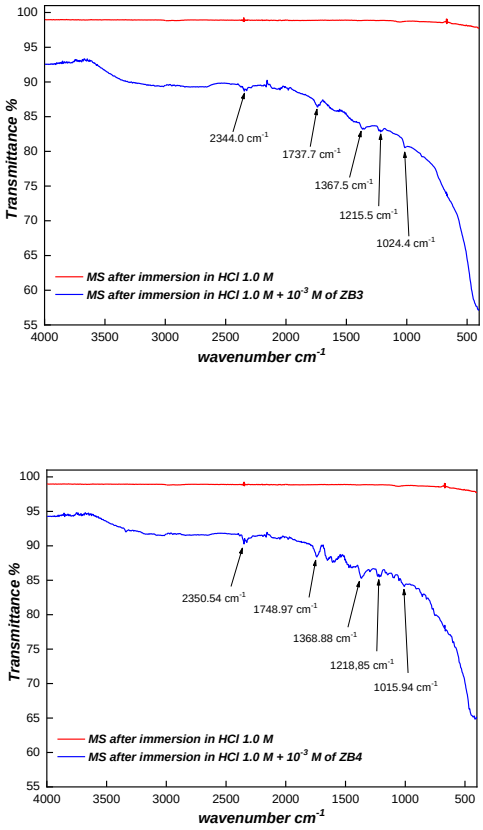


Figure S5. FT-IR spectrum of MS surface layer before and following the introduction of ZB3 and ZB4

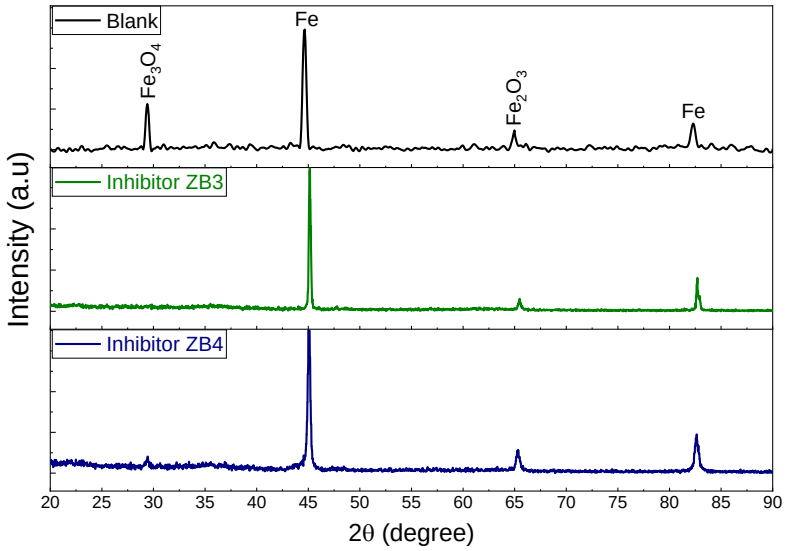


Figure S6. Diffractograms of the surface of m-steel after six hours of immersion in 1.0 M HCl (without & with 10^{-3}M of ZB3 and ZB4)

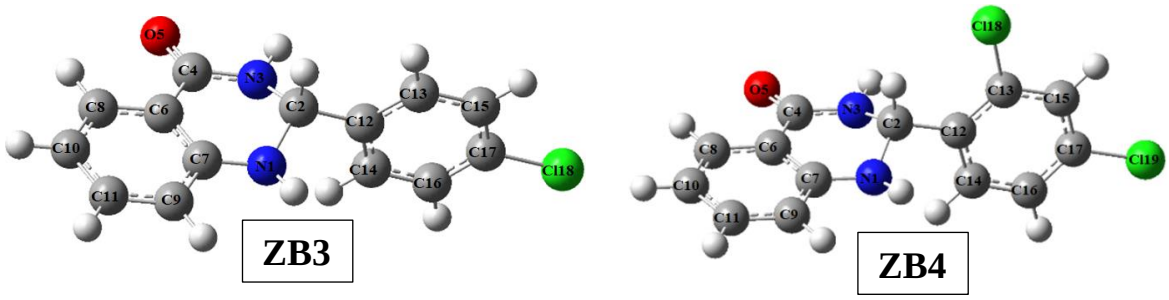


Figure S7. The picked geometrical parameters of the optimized investigated quinazolinone derivatives determined at B3LYP/6-31G(d,p) in gaseous (normal) and aqueous phases (underline)

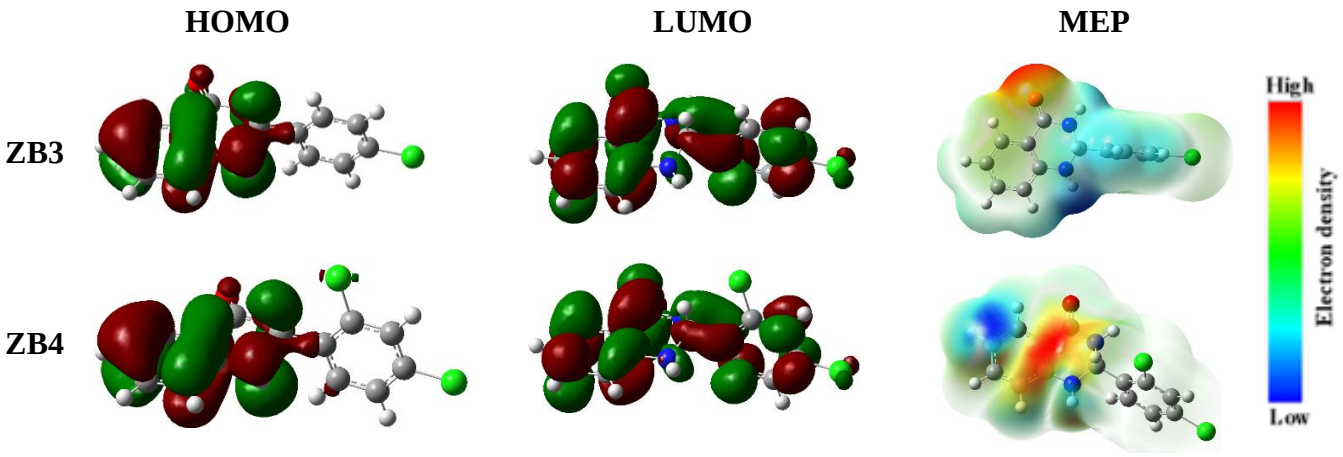


Figure S8. Electron density distributions of the HOMO and LUMO orbitals and MEP of ZB3 and ZB4 in solution in water at the B3LYP/6-31G(d,p) level of theory

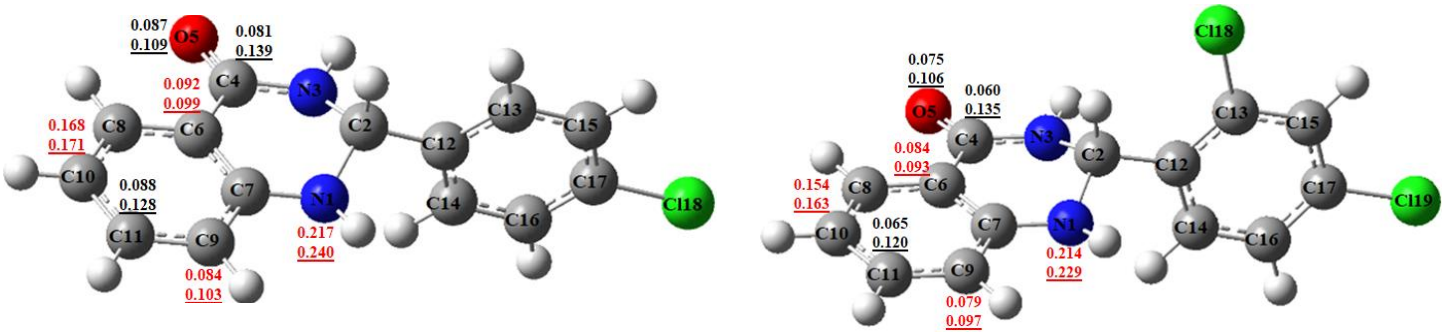


Figure S9. Fukui functions (f_k^+: black, f_k^-: red, normal: gas phase, underline: aqueous phase), the HOMO and the LUMO of ZB1 and ZB2 computed at B3LYP/6-31G(d,p) level of theory

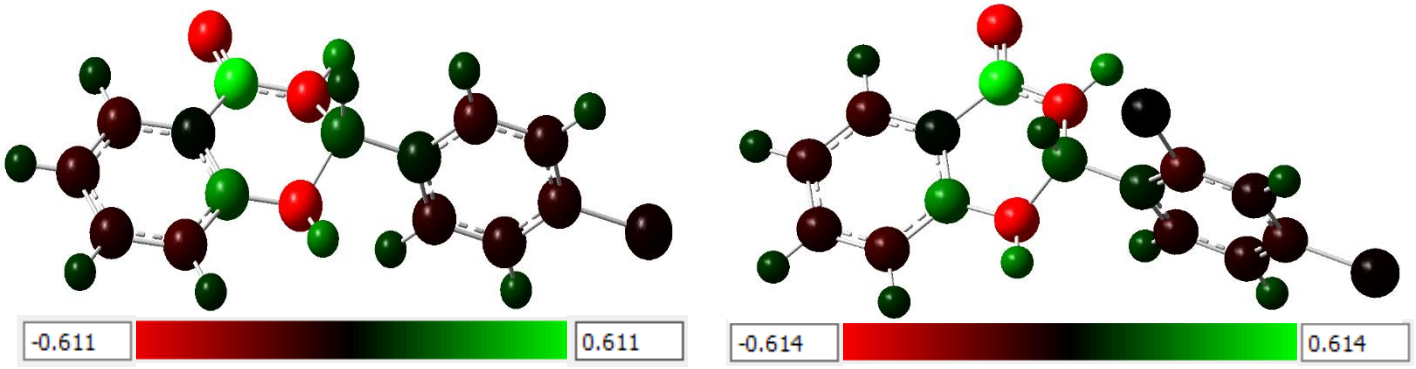


Figure S10. Mulliken charge distribution for quinazoline derivatives molecules calculated at the B3LYP/6++G(d,p) in aqueous medium

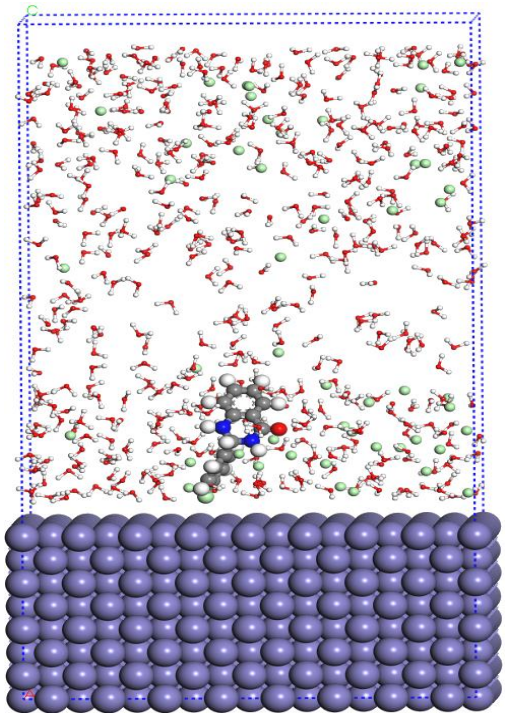
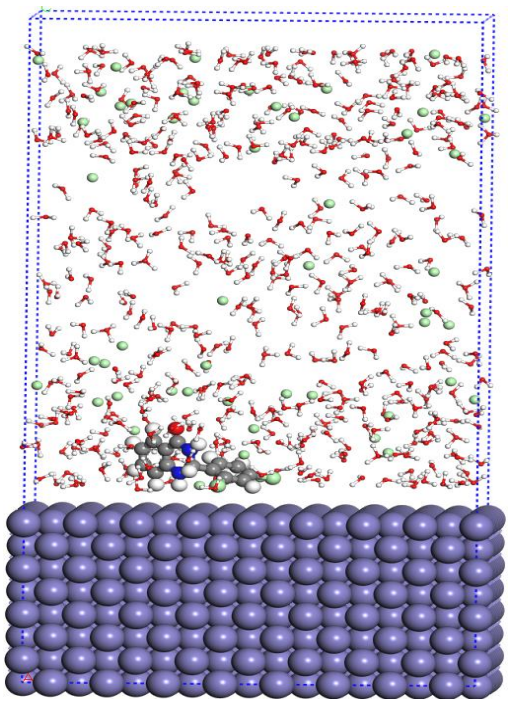
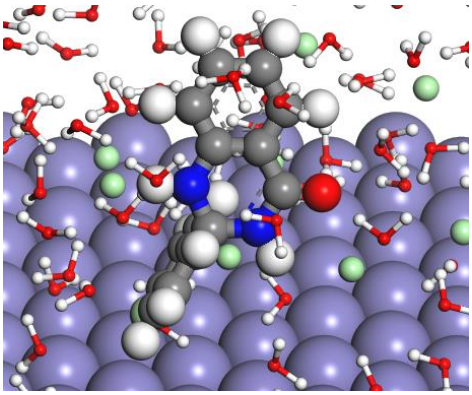
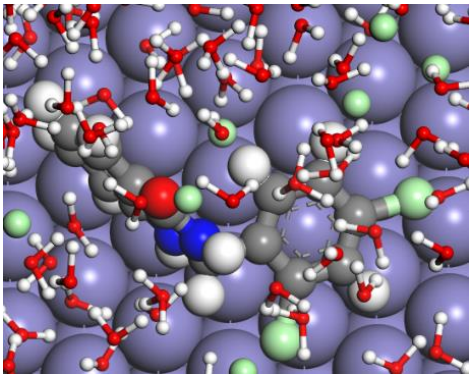
ZB3	ZB4
	
Side views	Side views
	
Top views	Top views

Figure S11. Side and top views of the most stable low energy configuration for the adsorption of the quinazolinone derivative molecules on the iron Fe(110) surface