

## **Supplemental section for RA-ART-01-2024-000158.R1**

**Title: An examination of the effectiveness of the expired drug Isoprinosine in preventing aluminum corrosion in alkaline solutions using both computational and experimental techniques**

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Figure S1: Simulated (□□□) and experimentally (◆◆◆) generated Nyquist plot for Al in 0.5 M NaOH in presence of 0.0112 M of Isoprinosine. (*inset*) The corresponding equivalent circuit was used in experimental impedance fit for Al in 0.5 M NaOH without and with different concentrations of Isoprinosine.

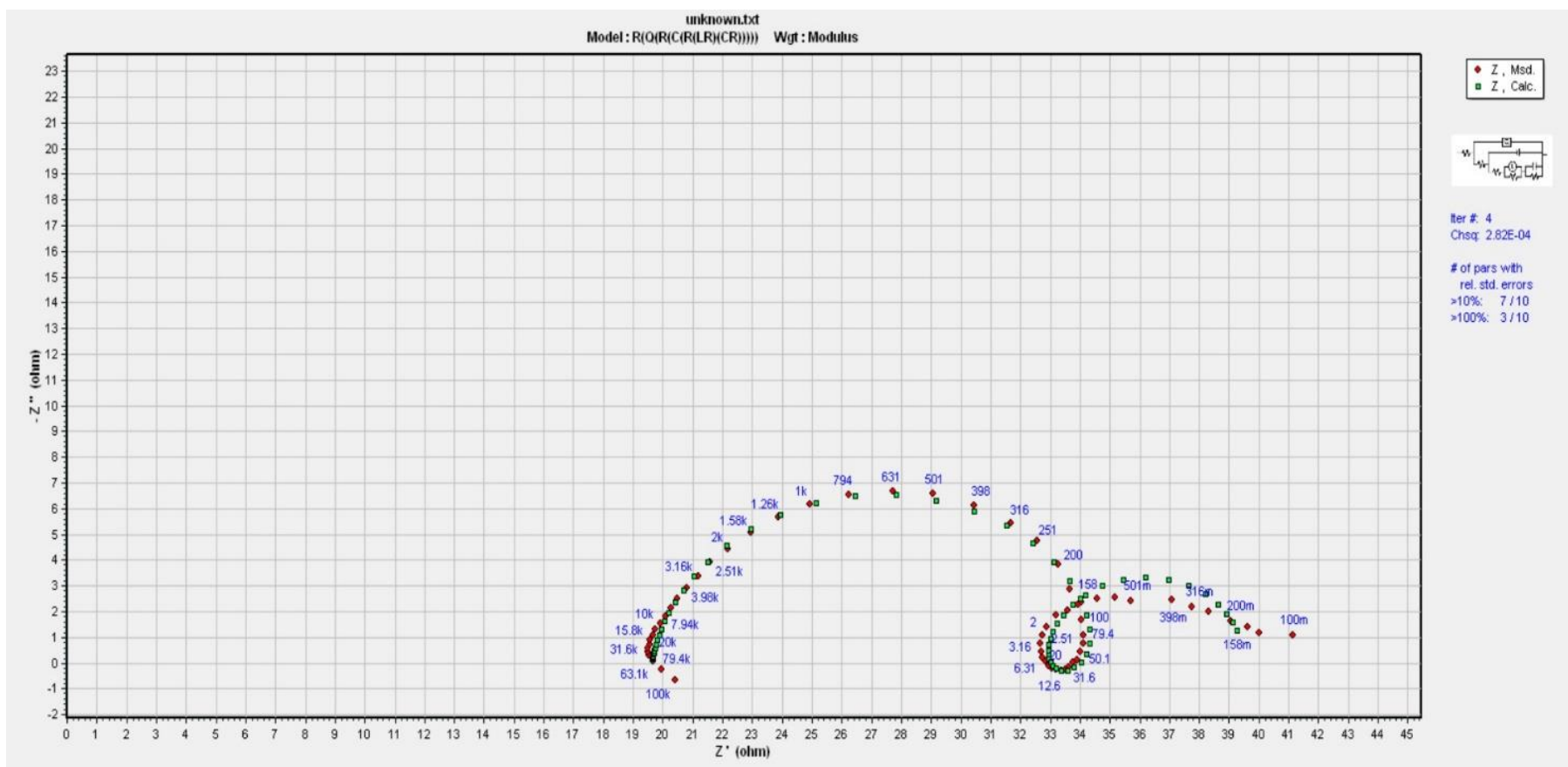
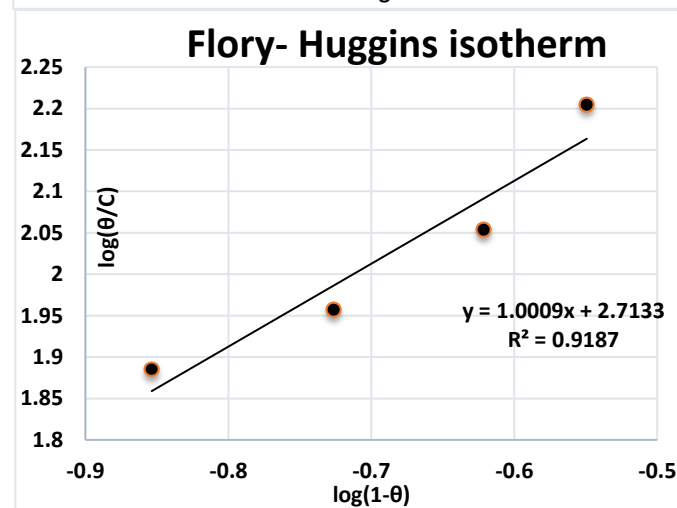
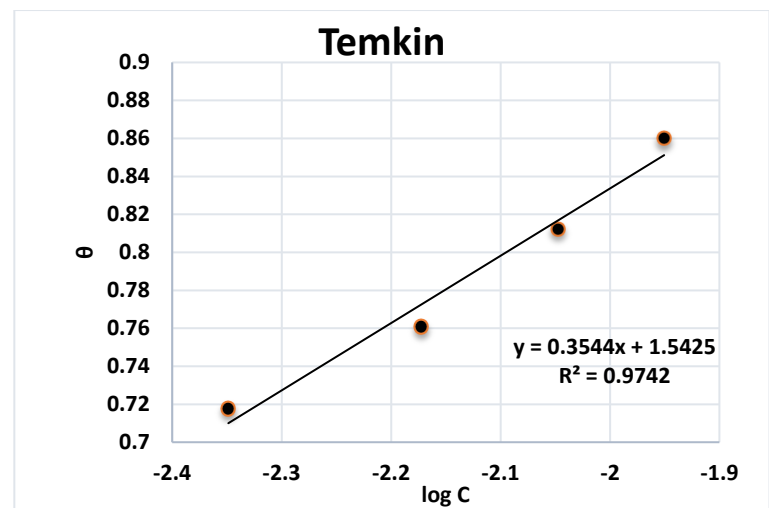
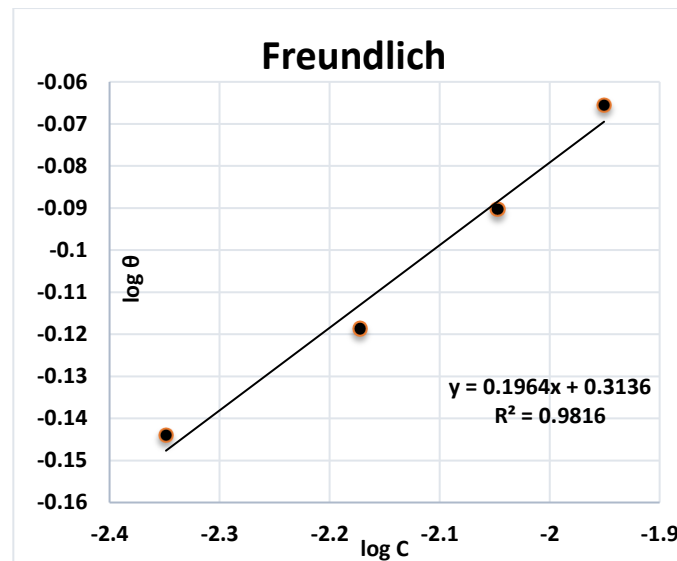
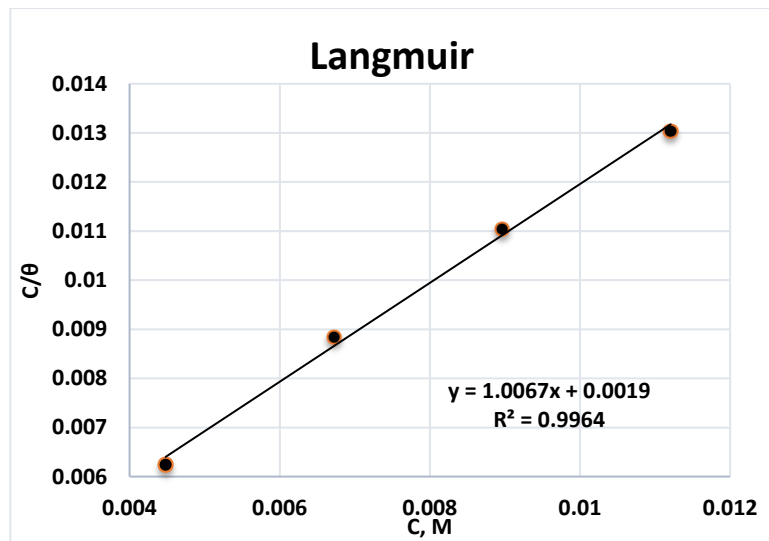


Figure S2: Adsorption isotherm for **Isoprinosine** on Aluminum electrode in 0.5 M NaOH.



**Figure S3:** Molecular dynamic simulations for the most favorable adsorption mode for **Isoprinosine** component on Al (110) surface.

