Rheological, Electrochemical, Surface, DFT and Molecular Dynamics Simulation Studies on the Anticorrosive Properties of New Epoxy Monomer Compound for Steel in 1 M HCl Solution

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**Supplementary Information**

**ER:** Brown viscous resin; $^1$H-NMR (300 MHz, CDCl$_3$): $\delta$ppm=2.38; 2.63 (dd, 2H, CH$_2$) (A,B), 2.77; 3.16 (m, 1H, CH oxirane) (X), 3.46 (dd, 2H, -N-CH$_2$) (C,D), 3.61 (dd, 2H, -CO(N)-CH$_2$) (A,B), 6.94; 7.71 (s, 4H aromatic) (Ar); FTIR (cm$^{-1}$): 3270 (residual hydroxyl and amine groups), 2978, 2883 (C-H vibrations), 1585, 1500, 1450 (1,2- substituted aromatic ring), 1654 (C=O amide), 1396, 1095, 1043 (C-O), 930, 880 (oxirane ring).

![Fig SI 1](image1.png) $^1$H NMR spectra of ER.

![Fig SI 2](image2.png) Mechanism of ring opening reaction of epoxides of ER in acid solution.
Fig. SI 3 The consequences of concentration on viscosity of ER/Ethanol at: 20, 40, 60 and 70 °C.

Fig. SI 4 Viscosity as a function of temperature of ER/Ethanol at various concentrations.
**Fig. SI 5** Arrhenius plots for the zero shear viscosity of concentrations of ER/Ethanol.

**Fig. SI 6** Equivalent circuit used for the analysis of the EIS data.
Fig. SI 7 Potentiodynamic polarization plots of carbon steel in 1 M HCl solution without and in the presence of $10^{-3}$ M of ER at varying temperatures.

Fig. SI 8 The relationship between $\ln (i_{\text{corr}})$ and $1/T$ for carbon steel in 1 M HCl solution without and in the presence of $10^{-3}$ M concentration of ER.
**Fig. SI 9** Transition state plots for carbon steel in 1 M HCl solution without and in the presence of 10^{-3} M concentration of ER.

**Fig. SI 10.** Langmuir adsorption isotherm plot of ER on the carbon steel surface at 298 K.
Fig. SI 11. EDX spectra of mild steel surface corroded in 1M HCl with and without ER.
Fig. SI 12. Graphical presentation of the calculated Fukui indices of ER and its protonated form ER⁺.
Table SI 1. Composition of the carbon steel.

|   | C     | Mn   | Si   | Al  | Cr | Mo | Ni | Cu   | Co   | V    | Fe  |
|---|-------|------|------|-----|----|----|----|------|------|------|-----|
|   | 0.11  | 0.47 | 0.24 | 0.03| 0.12| 0.02| 0.14| <0.001| <0.003| Balance |

Table SI 2. Name, abbreviation, chemical structure and analytical data of the synthesized compound.

| Inhibitor                          | Chemical structure | Analytical data                                                                 |
|------------------------------------|--------------------|---------------------------------------------------------------------------------|
| Tetracyclicyl-1,2-Aminobenzamide   | ER: Brown viscous resin, yield 92%; $^1$H-NMR (DMSO-d$_6$, 300 MHz): $\delta$ppm=2.38; 2.63 (dd, 2H, CH$_2$), 2.77; 3.16 (m, 1H, CH oxirane), 3.21; 3.46 (dd, 2H, -N-CH$_2$), 3.21; 3.36: 3.61 (dd, 2H, -CO(N)-CH$_2$), 6.94; 7.71 (s, 4H aromatic); FTIR (cm$^{-1}$): 3270 (residual hydroxyl and amine groups), 2978, 2883 (C-H vibrations), 1585, 1500, 1450 (1,2-substituted aromatic ring), 1654 (C=O amide), 1396, 1095, 1043 (C-O), 930, 880 (oxirane ring). | |

Table SI 3: The impact of temperature on the electrochemical parameters for carbon steel in 1 M HCl and 10$^{-3}$ M of ER.

| T (K) | $E_{corr}$ (mV/SCE) | $i_{corr}$ (µA/Cm$^2$) | $\eta$% |
|-------|---------------------|------------------------|--------|
| 298   | Blank - 473         | Blank 10$^{-3}$ M of ER | 10$^{-3}$ M of ER |
| 308   | - 459               | 1390                   | 69.70  |
| 318   | - 455               | 2700                   | 268.85 |
| 328   | - 453               | 4100                   | 546.82 |
Table SI 4: Activation parameters for carbon steel in 1 M HCl solution without and in the presence of ER.

|          | $E_a$ (kJ/mol) | $\Delta H_a$ (kJ/mol) | $\Delta S_a$ (J.mol$^{-1}$ K$^{-1}$) |
|----------|---------------|------------------------|---------------------------------------|
| Blank    | 41.94         | 39.30                  | -56.70                                |
| 10$^{-3}$ M of ER | 78.40         | 75.90                  | 38.07                                 |

Table SI 5: Calculated Quantum chemical parameters for epoxy compound and its protonated form obtained from DFT/B3LYB/6-311+G (d, p) in both gas phase and in solution.

| Energy (a.u.) | ER         | ER$^+$     | Gas   | ER         | ER$^+$     |
|---------------|------------|------------|-------|------------|------------|
| $\mu^*$      | 3.731      | 3.949      |       | 5.660      | 3.698      |
| $E_{HOMO}$ (eV) | -6.385    | -6.615     | -6.338 | -6.511     |
| $E_{LUMO}$ (eV) | -0.968    | -1.208     | -0.881 | -1.060     |
| I             | 6.385      | 6.615      | 6.338  | 6.511      |
| A             | 0.968      | 1.208      | 0.881  | 1.060      |
| $\Delta E$   | 5.417      | 5.407      | 5.457  | 5.451      |
| $\chi$       | 3.676      | 3.912      | 3.609  | 3.785      |
| $\eta$       | 2.709      | 2.704      | 2.728  | 2.726      |
| $\sigma$     | 0.369      | 0.370      | 0.367  | 0.367      |
| $\omega$     | 2.709      | 2.704      | 2.728  | 2.726      |
| $\Delta N100$ | 0.043      | 0.000      | 0.043  | 0.000      |
| $\Delta N110$ | 0.211      | 0.168      | 0.211  | 0.168      |
| $\Delta N111$ | 0.038      | -0.006     | 0.038  | -0.006     |
| $\Delta \psi$ | 1.020      | 0.882      | 1.054  | 0.948      |
| $\Delta E_{b-d}$ | -0.677    | -0.676     | -0.682 | -0.681     |