LIST OF TABLES

	Page No.
Table 1.1: Various types of adsorption isotherms	41
Table 1.2: Literature survey: DFT methods in corrosion inhibition	49
Table 2.1.1: The molecular structure and IUPAC name of synthesized Pyranopyrazoles	63
Table 2.1.2: The molecular structure and IUPAC name of synthesized pyridine based Schiff bases derivatives.	66
Table 2.1.3: The molecular structure and IUPAC name of synthesized Imidazole derivatives.	69
Table 2.1.4: The molecular structure and IUPAC name of synthesized Pyrazolo-pyridine derivatives	71
Table 3.1.1: IUPAC name, molecular structure, abbreviation and analytical data of the studied inhibitor molecules (EPPs)	82
Table 3.1.2: The gravimetric measurement parameters obtained for mild steel in 1 M HCl containing different concentrations of EPPs	86
Table 3.1.3: Variation of C_R and η % with temperature in absence and presence of optimum concentration of EPPs in 1M HCl	88
Table 3.1.4: The values of $K_{\rm ads}$, $\Delta G^{\circ}_{\rm ads}$ and $E_{\rm a}$ for mild steel in the absence and presence of optimum concentration of EPPs in 1M HCl at 308K	91
Table 3.1.5: Potentiodynamic polarization parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100 mg L ⁻¹) of EPPs at 308K	95

Table 3.1.6: Electrochemical impedance parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100 mg L ⁻¹) of EPPs at 308K	96
Table 3.1.7: Quantum chemical parameters derived from the B3LYP/6-31+G (d,p) method of the studied compounds.	103
Table 3.1.8: Calculated Fukui functions for the studied inhibitor molecules in neutral forms	106
Table 3.1.9: Outputs and descriptors calculated by the Monte Carlo simulation for the most stable adsorption configurations of EPP-1, EPP-2 and EPP-3 on Fe (110) surface (all units in kJ/mol) in vacuum phase and aqueous phase.	110
Table 3.2.1: molecular structure and analytical data of DAPs	112
Table 3.2.2: gravimetric measurements (±SD) for MS in the Absence and Presence of DAPs in 1 M HCl at 308 K	115
Table 3.2.3: Thermodynamic parameters for the adsorption of inhibitor on mild steel in 1 M HCl at optimum concentration (40 mgL ⁻¹) of DAPs at 308 K	118
Table 3.2.4: Electrochemical impedance parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (40 mg L ⁻¹) of DAPs at 308K	124
Table 3.2.5: Potentiodynamic polarization parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (40 mg L ⁻¹) of DAPs at 308K	125
Table 3.2.6: Calculated quantum chemical parameters for DAPs derived from the B3LYP/6-31+G(d,p)method	134
Table 3.2.7: Calculated Fukui functions for the studied neutral inhibitor molecules	134
Table 3.2.8: Interaction energies between the inhibitors and Fe (110) surface	138

(kJ/mol)

Table 3.3.1: IUPAC name, molecular structure, abbreviation and analytical data of the studied inhibitor molecules (IMs)	141
Table 3.3.2: The weight loss parameters obtained for mild steel in 1 M HCl containing different concentrations of IMs	143
Table 3.3.3: Thermodynamic parameters for mild steel dissolution in 1M HCl in the absence and presence of optimum (100 mgL ⁻¹) concentration of inhibitors	145
Table 3.3.4: Adsorption parameters for IMs calculated from the different isotherms for mild steel in 1M HCl solution.	147
Table 3.3.5: Electrochemical impedance parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100 mg L ⁻¹) of inhibitors	149
Table 3.3.6: Potentiodynamic polarization parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100mgL ⁻¹) of inhibitors	153
Table 3.3.7: Calculated quantum chemical parameters of neutral and protonated IMs in gas phase.	160
Table 3.3.8. Selected energy parameters obtained from MD simulations for adsorption of inhibitors on Fe (110) surface	163
Table 3.4.1 IUPAC Name, molecular structure and abbreviation of the condensed Pyrazolopyridine used	167
Table 3.4.2: Corrosion parameters for the mild steel in 1 M HCl containing various concentrations of the PPs at 308 K obtained from gravimetric measurements	169
Table 3.4.3: Thermodynamic parameters for the adsorption of inhibitor on mild steel in 1M HCl at optimum concentration of PPs	171

Table 3.4.4: Adsorption parameters for PPs calculated from different adsorption	172
isotherm for mild steel in 1M HCl solution at 308K	
Table 3.4.5: Electrochemical impedance parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100 mg L ⁻¹) of PPs at 308K	177
Table 3.4.6: Potentiodynamic polarization parameters (±SD) for mild steel in 1M HCl in absence and presence of optimum concentration (100 mg L ⁻¹) of PPs at 308K	178
Table 3.4.7: Calculated quantum chemical parameters of neutral and protonated PPs DFT (6-31G, d, p)	184
Table 3.4.8: Calculated Fukui functions for the studied inhibitor molecules in neutral	188
Table 3.4.9: Interaction energies between the inhibitors and Fe (110) surface (kJ/mol) in gas phase	190
Table 3.4.10. The diffusion coefficient of Cl^- and $H O^+$ at 303 K	194

ABBREVIATIONS

 η % = Percentage of inhibition efficiency

 $C_{\rm R}$ = Corrosion rate (mgcm⁻²h⁻¹)

 $C_{\rm R}^{\rm o}$ = Corrosion rate in uninhibited system (mgcm⁻²h⁻¹)

 $C_{\rm R}^{\rm i}$ = Corrosion rate in inhibited system (mgcm⁻²h⁻¹)