

**SUPPLEMENTARY INFORMATION**

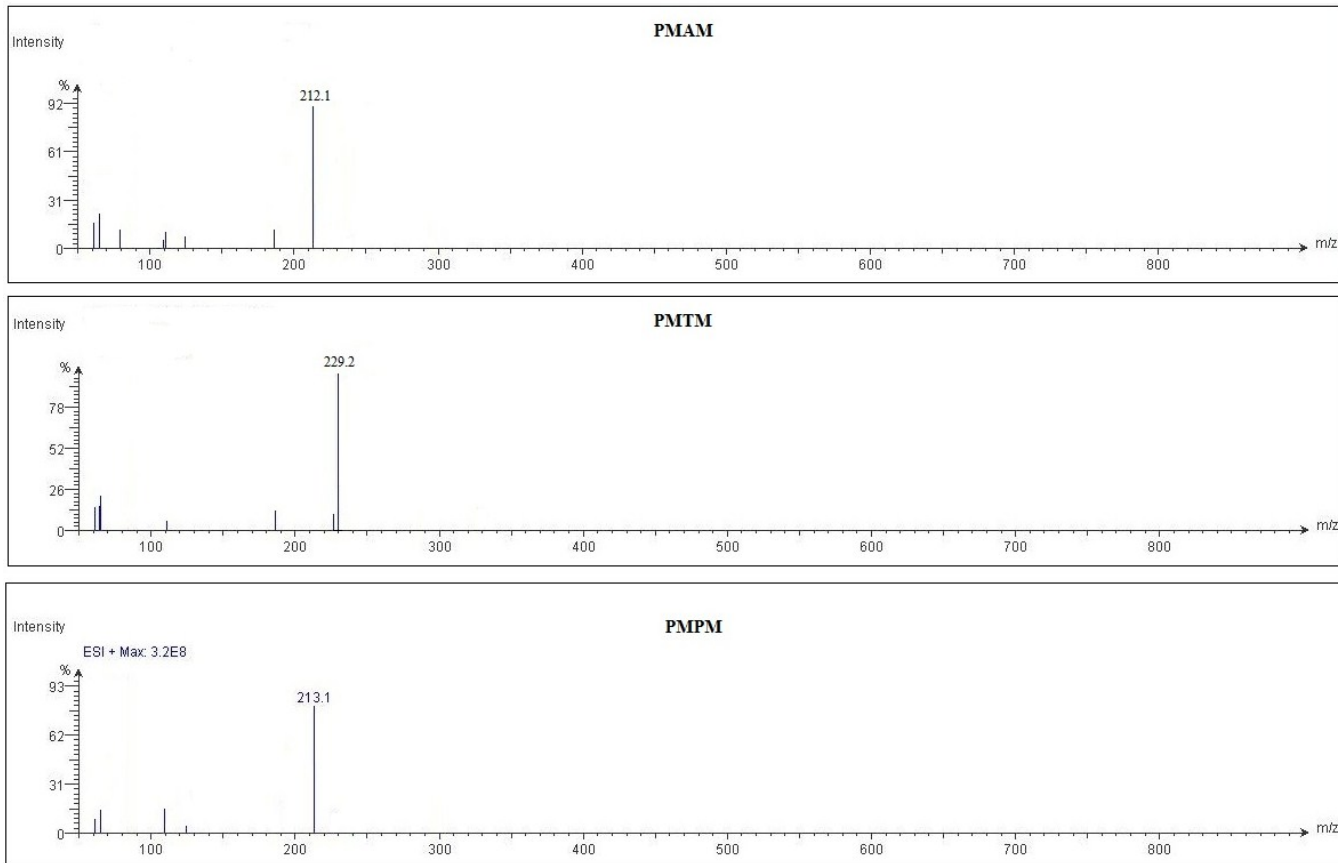
**Evaluating corrosion inhibition property of some Schiff bases for mild steel in 1M HCl:  
competitive effect of heteroatom and stereochemical conformation of the molecule**

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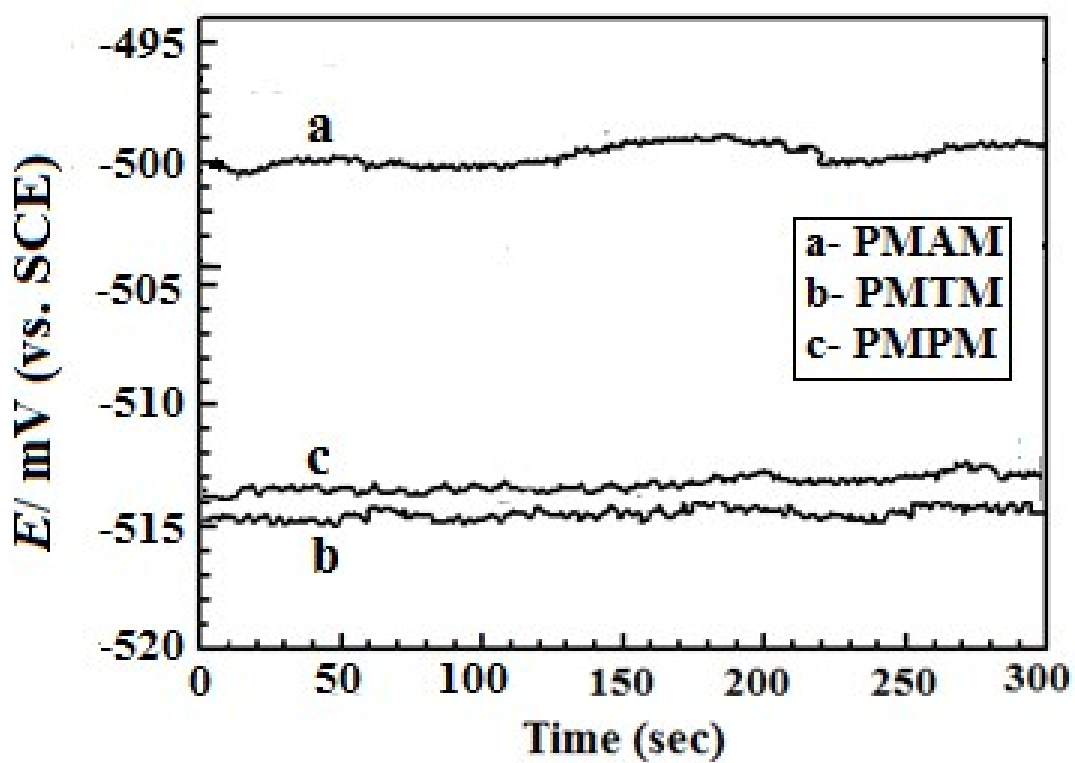
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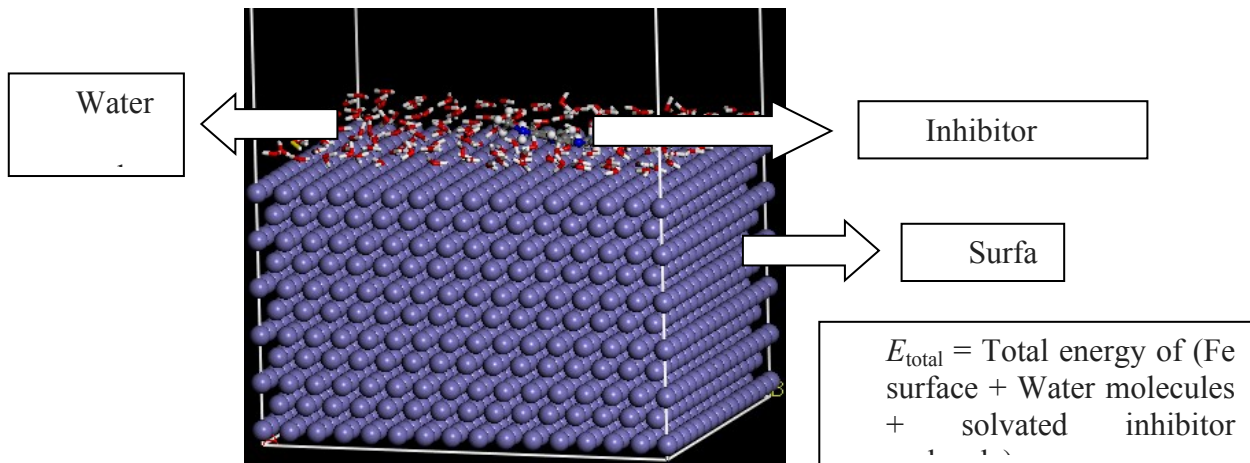
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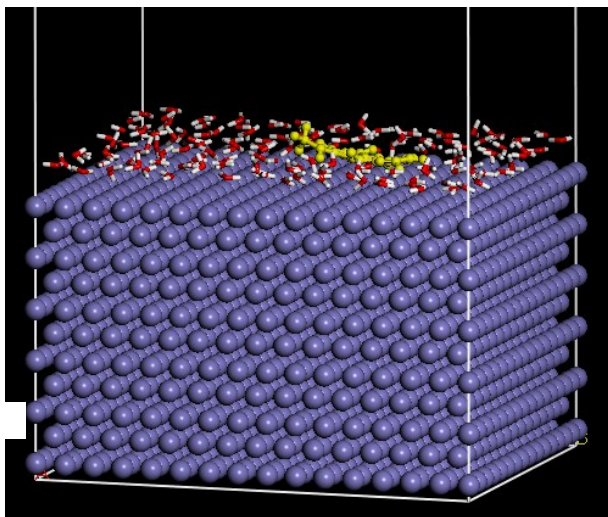
**Fig. S1** ESI-MS spectrum of of PMAM, PMTM and PMPM inhibitors in methanol.



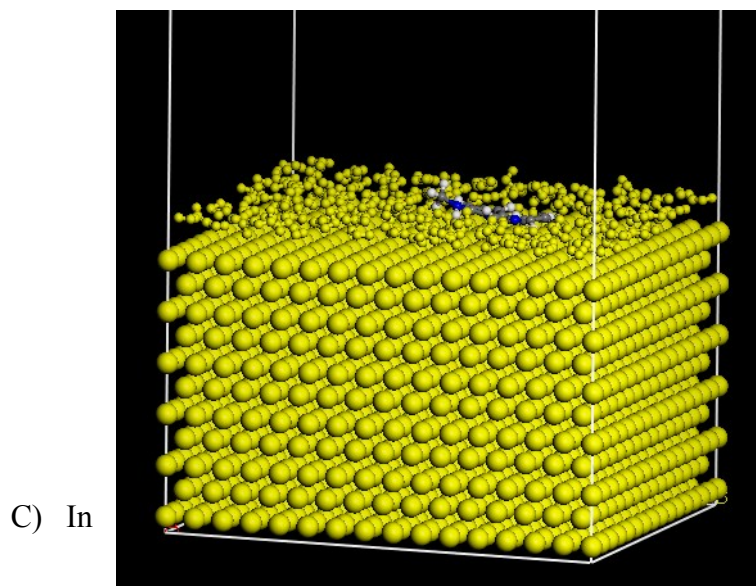
**Fig. S2.** Variation of rest potential with time for mild steel in 1M HCl having 10 mM Schiff-base after an exposure for 45 mins.



A) Box 1: At equilibrated state, inhibitor molecule is in solvated form.



B) Fe surface and solvent water molecules are selected from box 1 (solvated inhibitor is not selected and is reflected in yellow impression) to obtain  $E_{\text{surface+water}}$ .



solvent stabilized inhibitor molecule present in box 1 will result into  $E_{\text{inh(solv)}}$ .

**Fig. S3 (A-C).** Pictorial representation for deriving the energy components following MD simulation experimentation.

**Fig. S4 A**

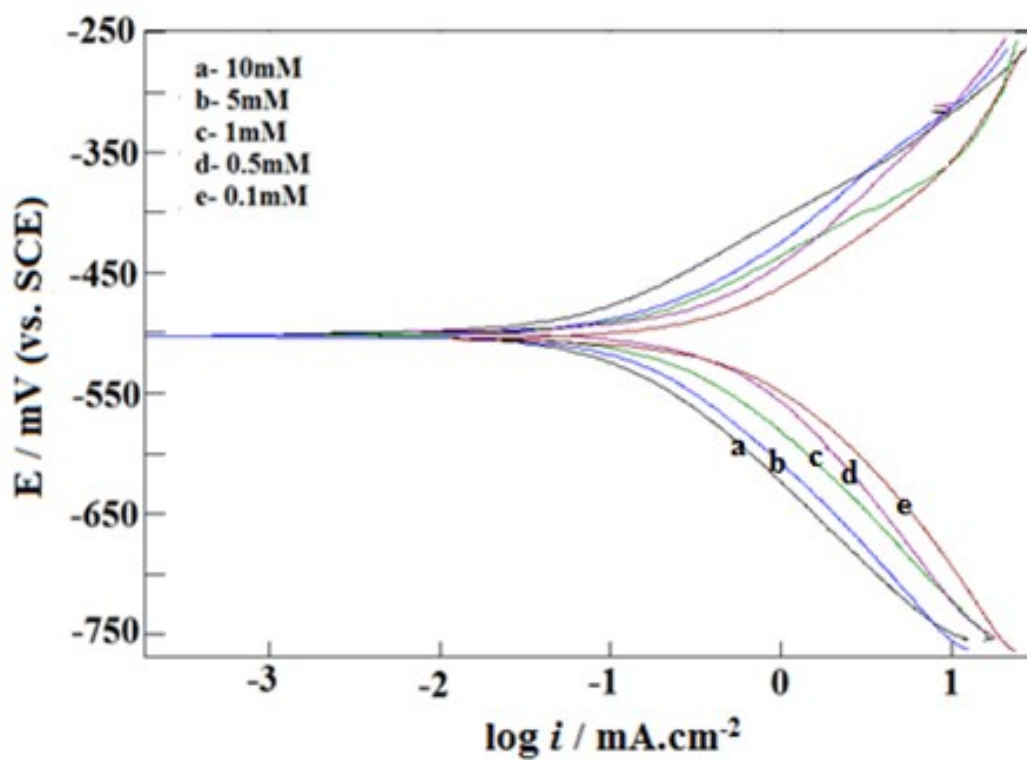


Fig. S4 B

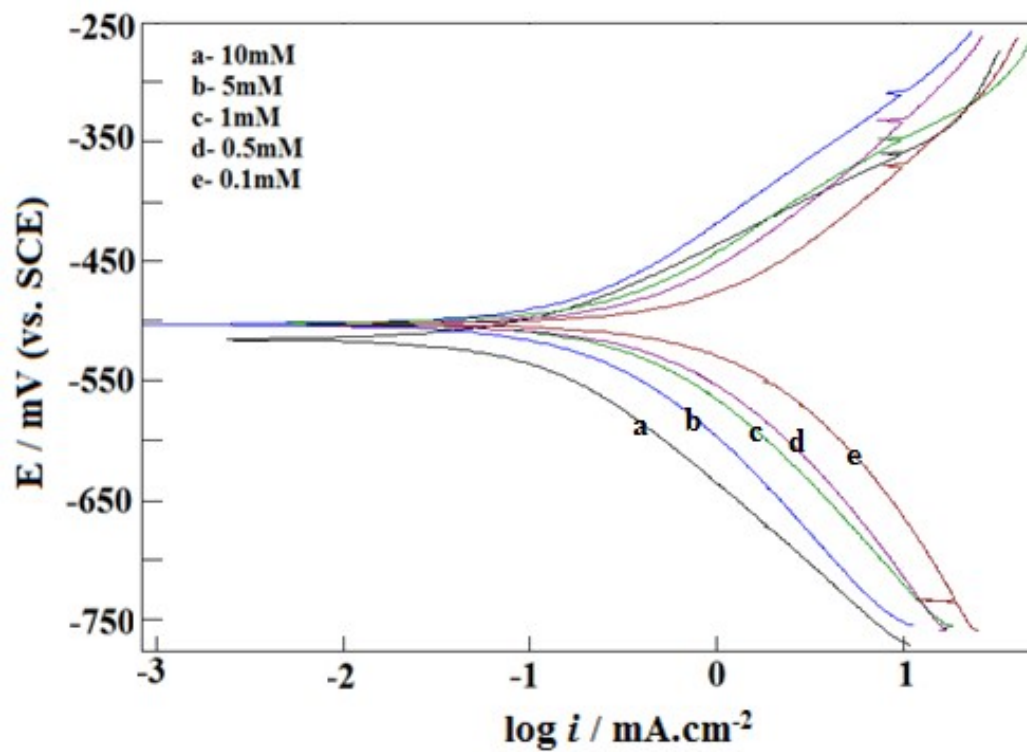
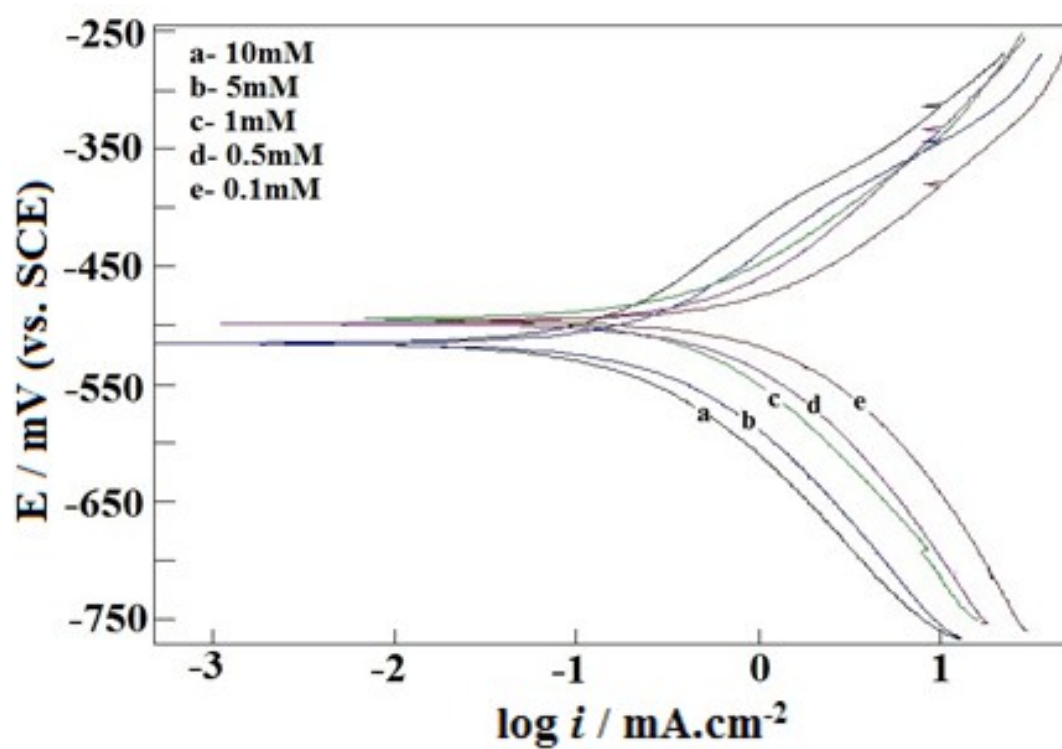
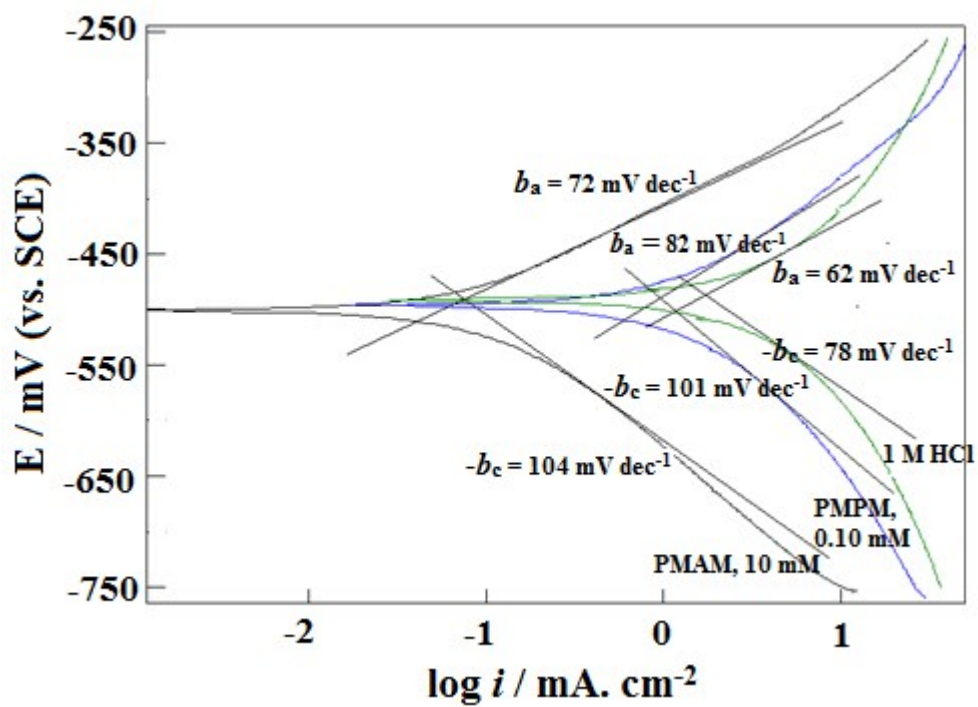


Fig.  
C



**Fig. S4 (A-C).** Potentiodynamic polarization curves for mild steel in 1M HCl in presence of (A) PMAM, (B) PMTM and (C) PMPM inhibitors.



**Fig. S5.** Fitting of the potentiodynamic polarization curves for mild steel in 1M HCl and in the presence of PMPM (0.10 mM) and PMAM (10mM) showing the value of Tafel slopes.

**Fig. S6 A**



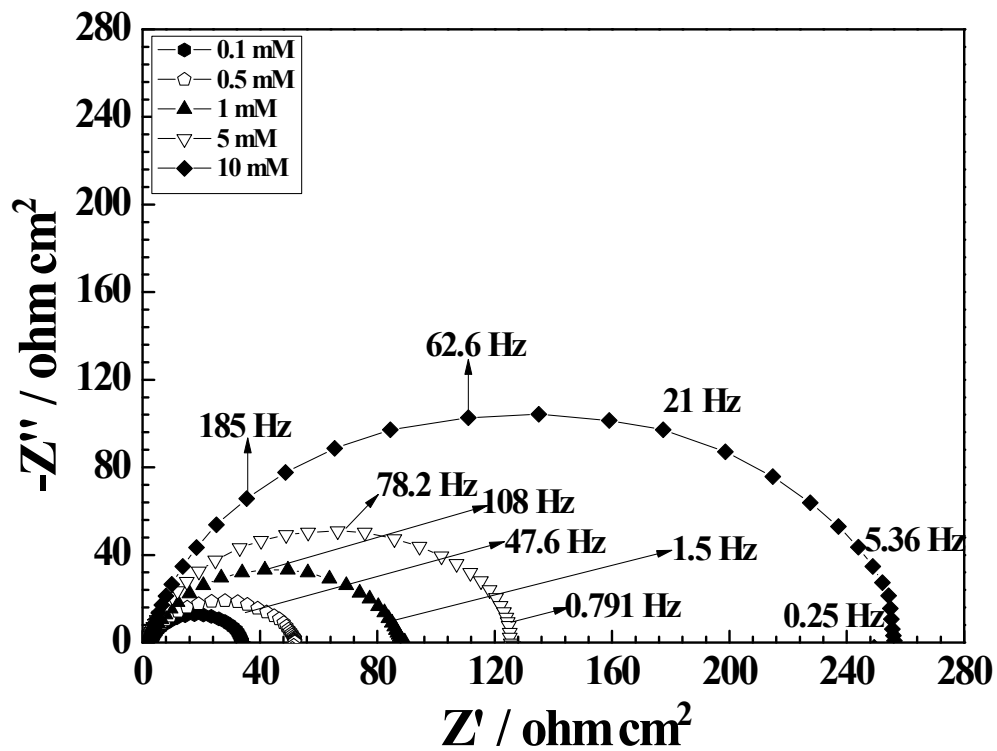


Fig. S6 B

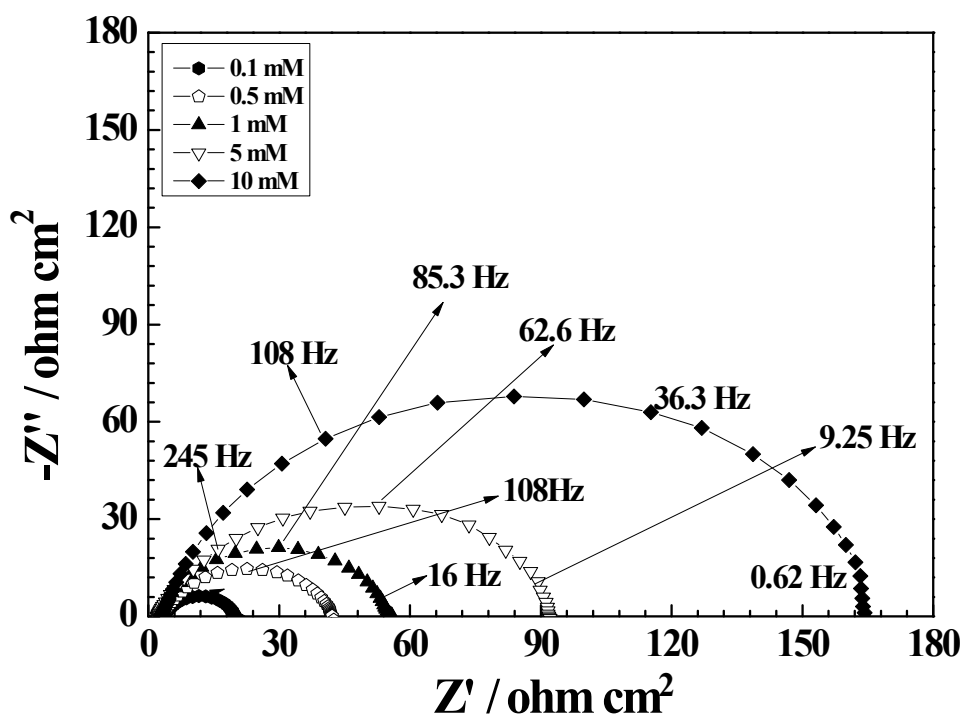


Fig. S6 C

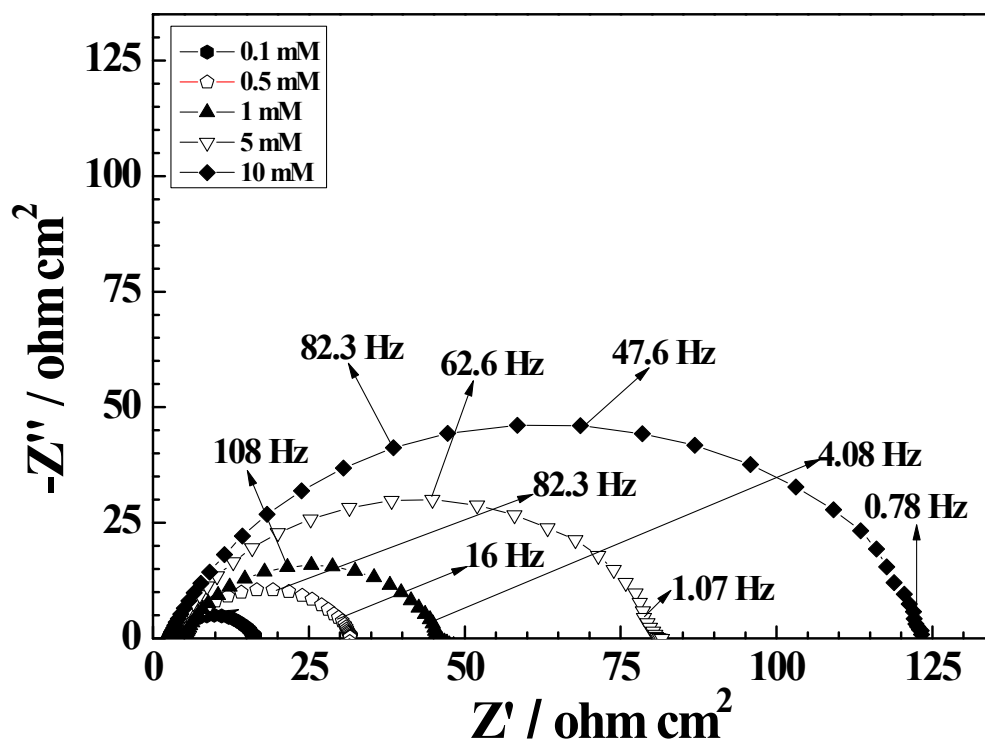


Fig. S6 (A-C). Nyquist plots of mild steel in 1M HCl containing (A) PMAM, (B) PMTM and (C) PMPM inhibitors.

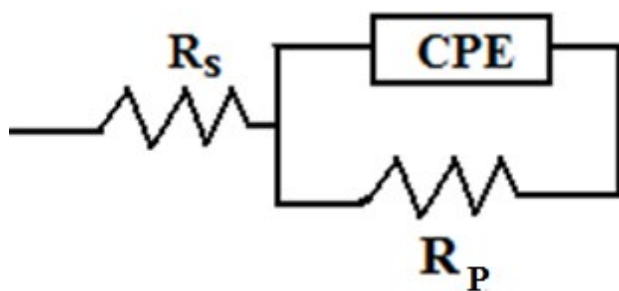


Fig. S7 Equivalent circuit model used to fit the impedance spectra.

Fig. S8 A

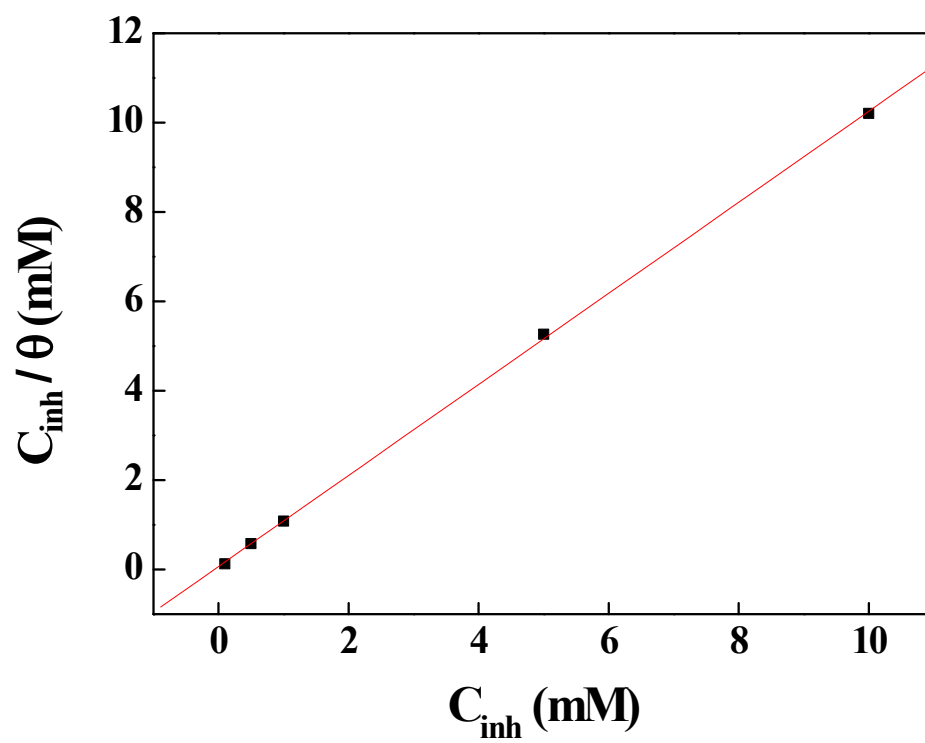


Fig. S8 B

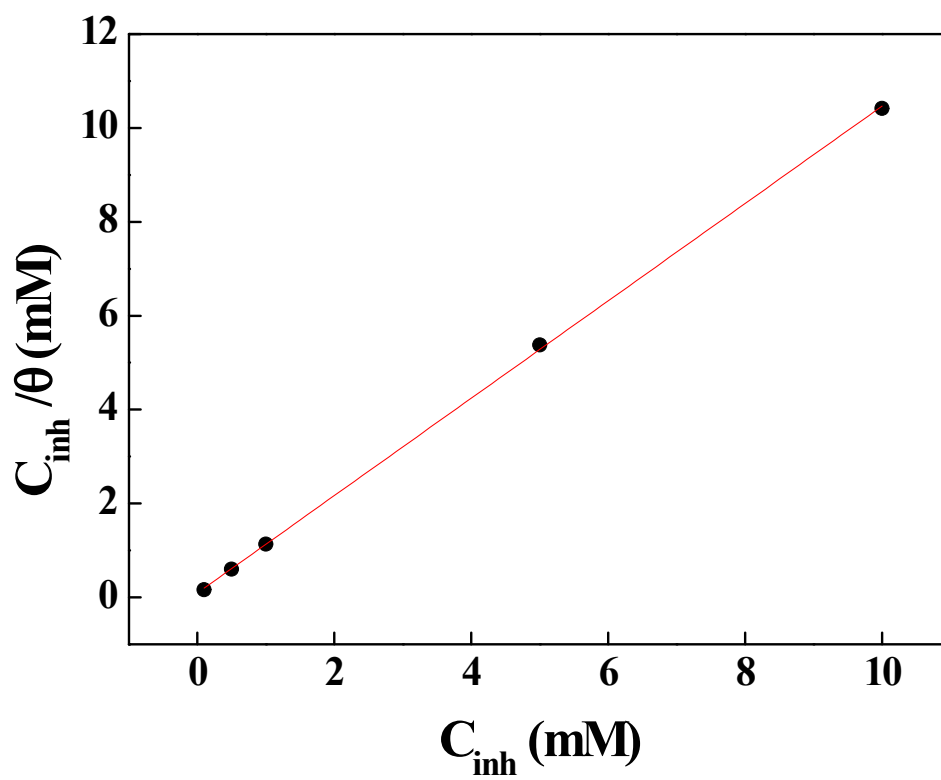


Fig. S8 C

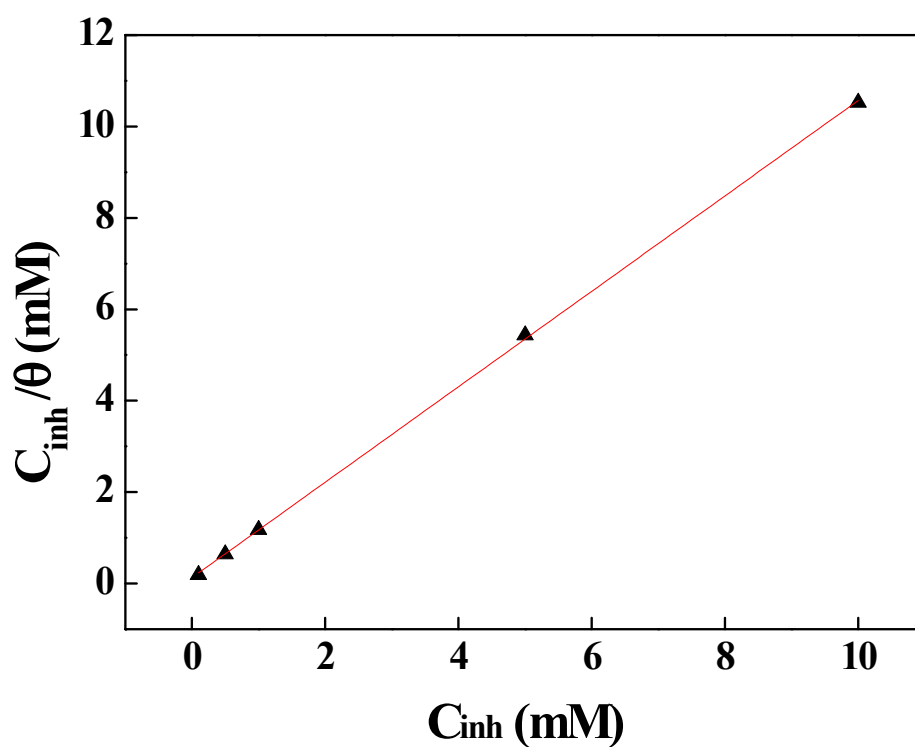


Fig. S8 (A-C). Langmuir adsorption plots for mild steel in 1M HCl at 303K containing different concentration of (A) PMAM, (B) PMTM and (C) PMPM.

**Table S1.** Calculated Fukui functions for the three inhibitor molecules.

Atom	PMAM		PMTM		PMPM	
	$f_k^+$	$f_k^-$	$f_k^+$	$f_k^-$	$f_k^+$	$f_k^-$
C (1)	0.044	0.014	0.046	0.009	0.045	0.021
C (2)	0.077	0.022	0.080	0.014	0.079	0.030
C (3)	0.058	0.013	0.059	0.008	0.058	0.017
C (4)	0.050	0.019	0.053	0.012	0.053	0.027
C (5)	0.058	0.009	0.057	0.005	0.057	0.014
N (6)	0.073	0.017	0.075	0.011	0.075	0.027
C (7)	0.098	0.051	0.105	0.029	0.109	0.059
N (8)	0.092	0.034	0.094	0.016	0.100	0.082
C (9)	0.009	0.031	0.008	0.046	0.008	0.019
C (10)	0.032	0.038	0.028	0.030	0.032	0.048
C (11)	0.024	0.087	0.022	0.048	0.023	0.072
C (12)	0.039	0.048	0.037	0.038	0.040	0.086
C (13)	0.018	0.062	0.016	0.033	0.018	0.071
C (14)	0.026	0.055	0.022	0.029	0.025	0.068
C (15)	0.024	0.059	0.020	0.039	0.022	0.045
N (16)	0.023	0.136	–	–	–	–
S (16)	–	–	0.040	0.403	–	–
O (16)	–	–	–	–	0.014	0.061