Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2015

:Supplementary File:

Adsorption and corrosion inhibition effect of Schiff base molecules on the mild steel surface in 1 M HCl medium: A combined experimental and theoretical approach

Sourav Kr. Saha,[ab] Alokdut Dutta,[c] Pritam Ghosh,[a] Dipankar Sukul[c] and Priyabrata Banerjee[ab]*

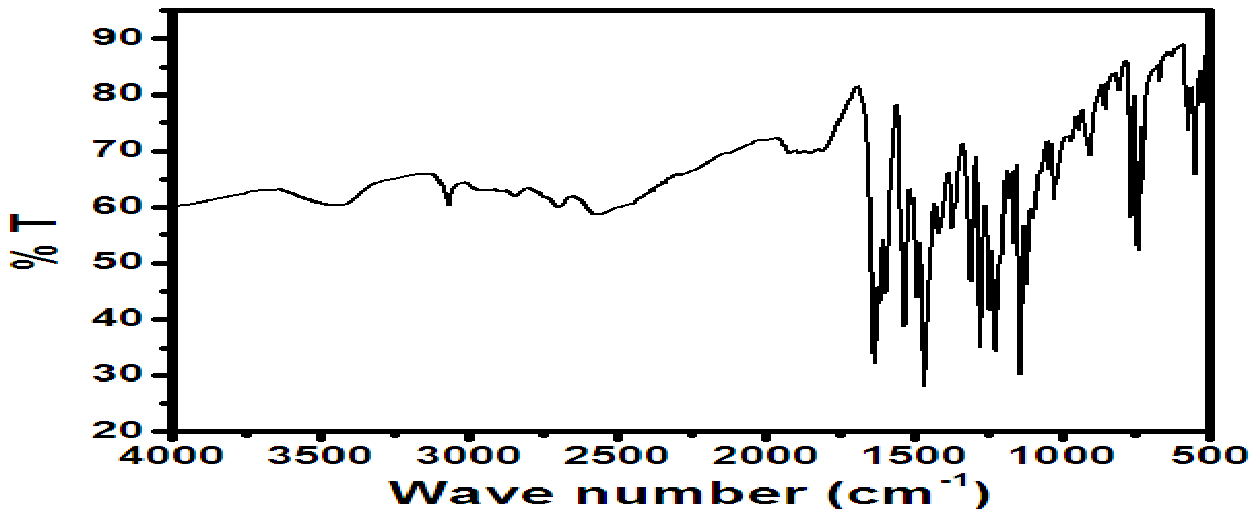

Fig. S1 FTIR spectrum of L[1].

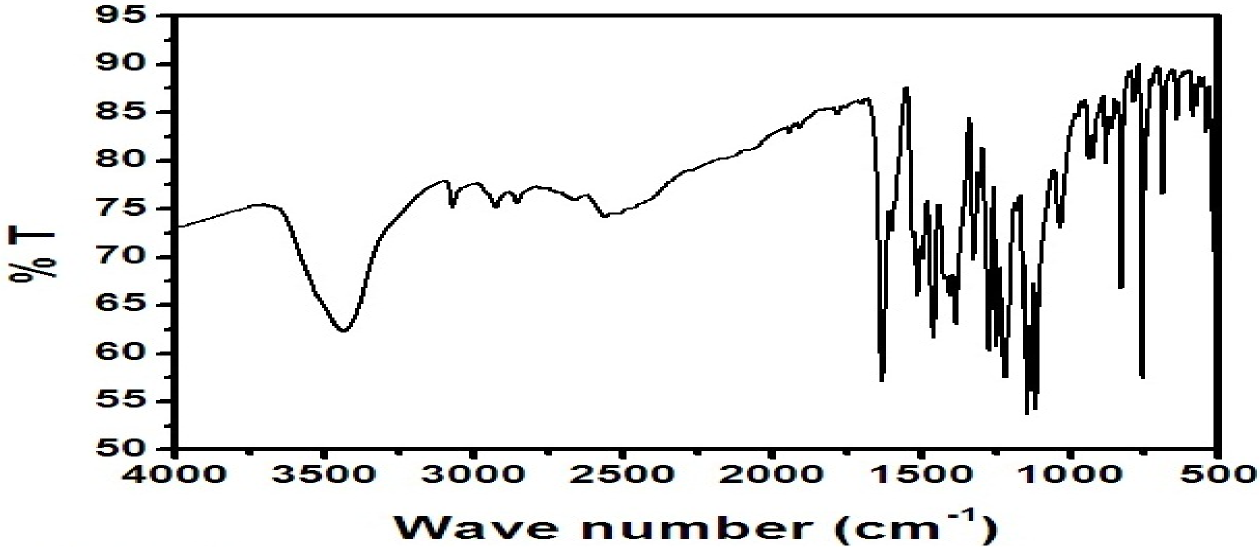

Fig. S2 FTIR spectrum of L[2].

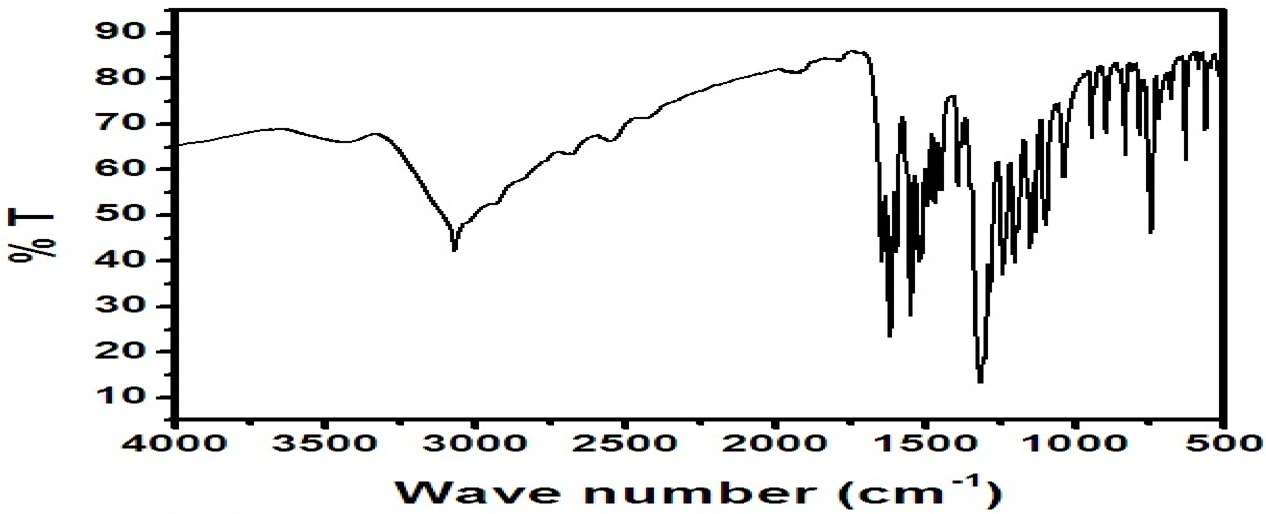

Fig. S3 FTIR spectrum of L[3].

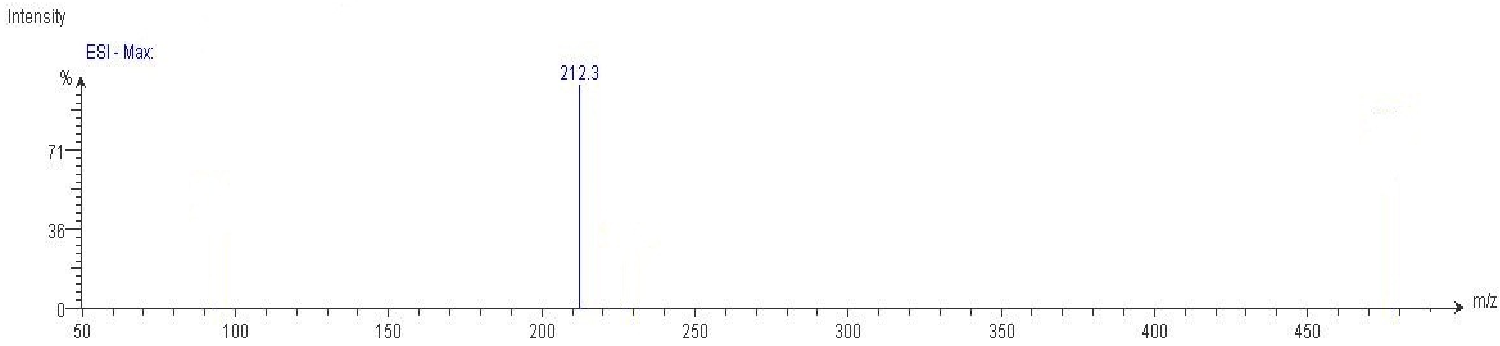

Fig. S4 ESI-MS spectrum of L^1 in methanol.

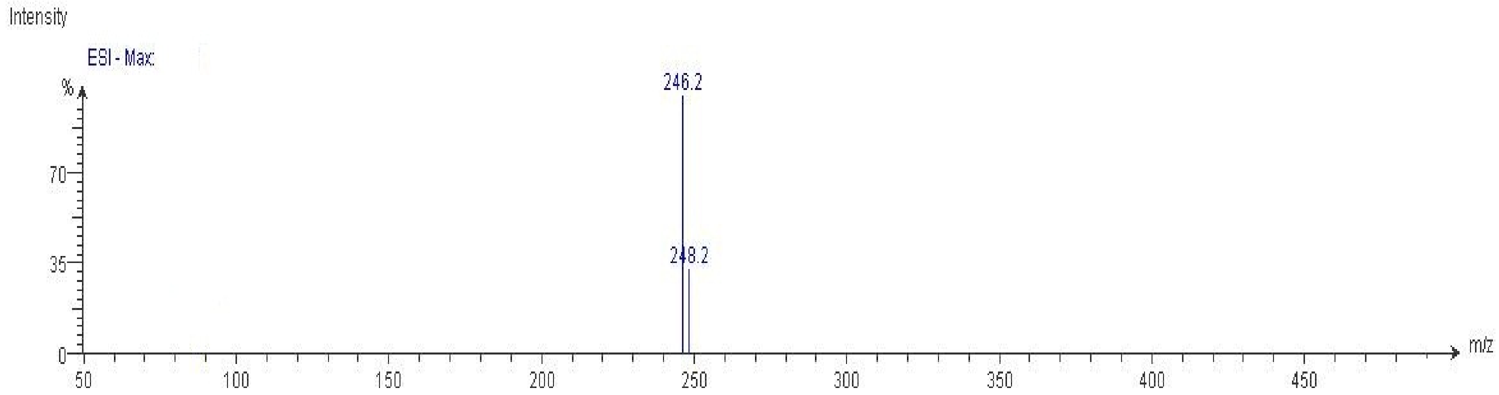

Fig. S5 ESI-MS spectrum of L^2 in methanol.

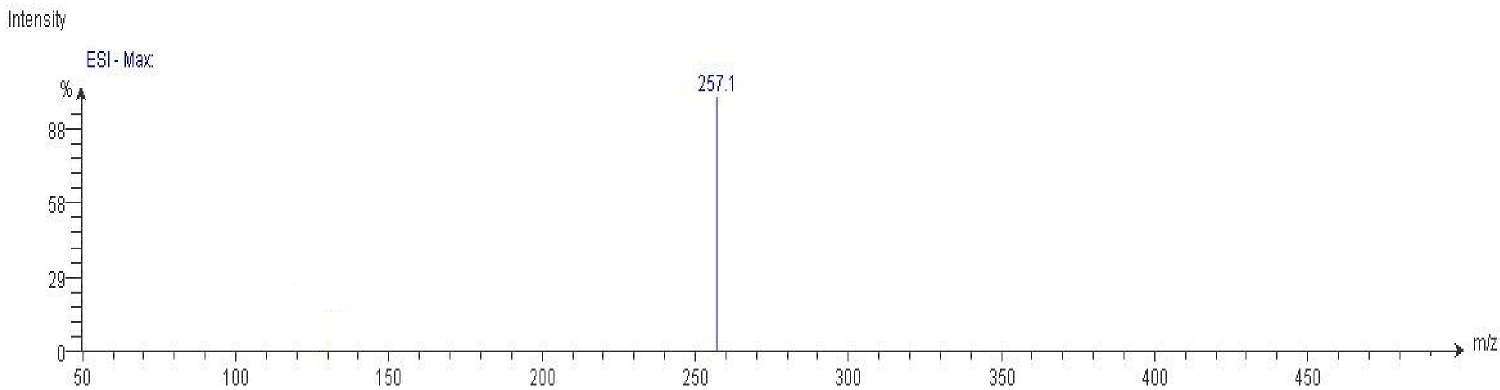

Fig. S6 ESI-MS spectrum of L^3 in methanol.

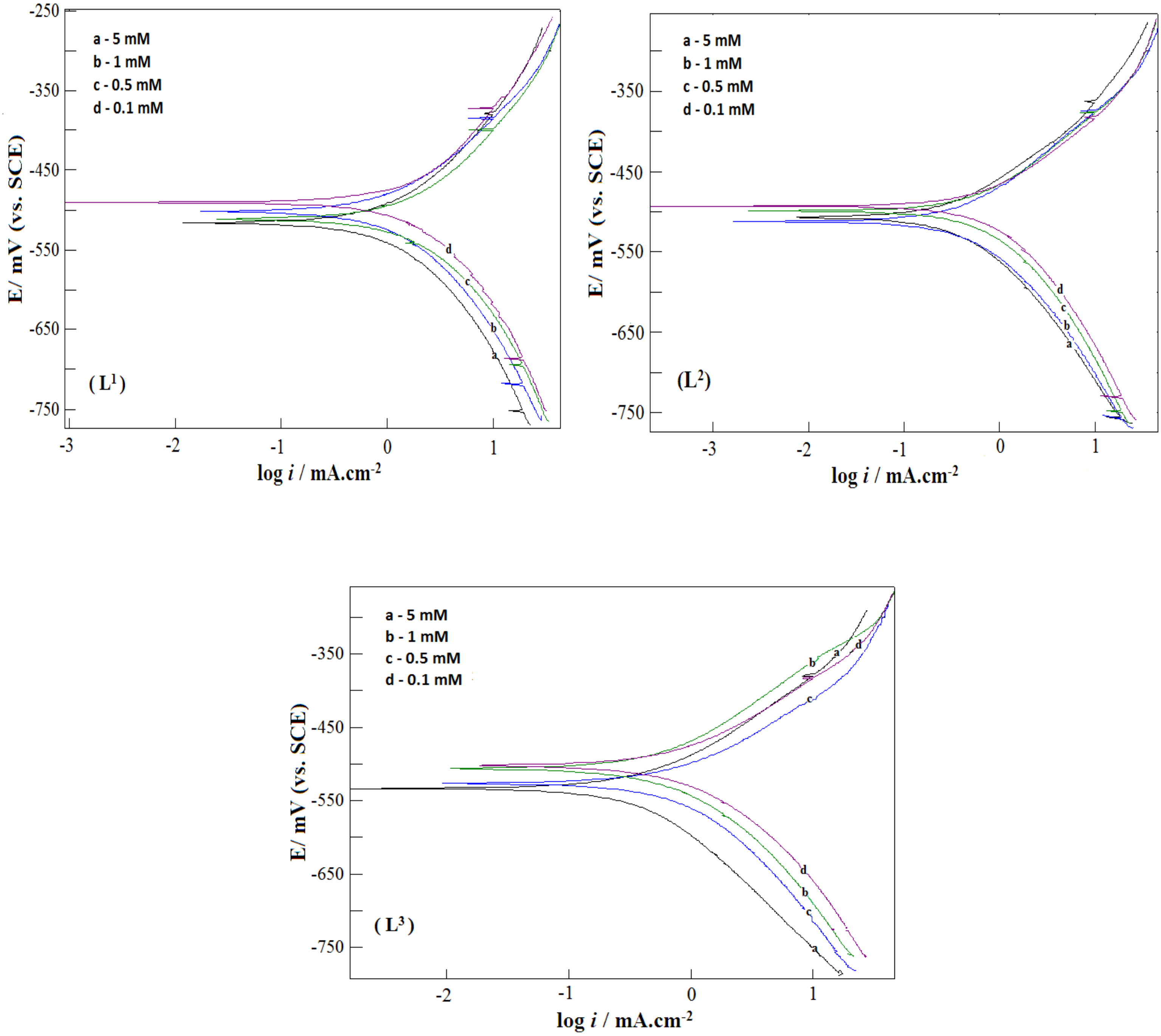

Fig. S7 Potentiodynamics polarization curves of mild steel in 1 M HCl solution in the presence of different concentration of Schiff bases at 27^{0}C.

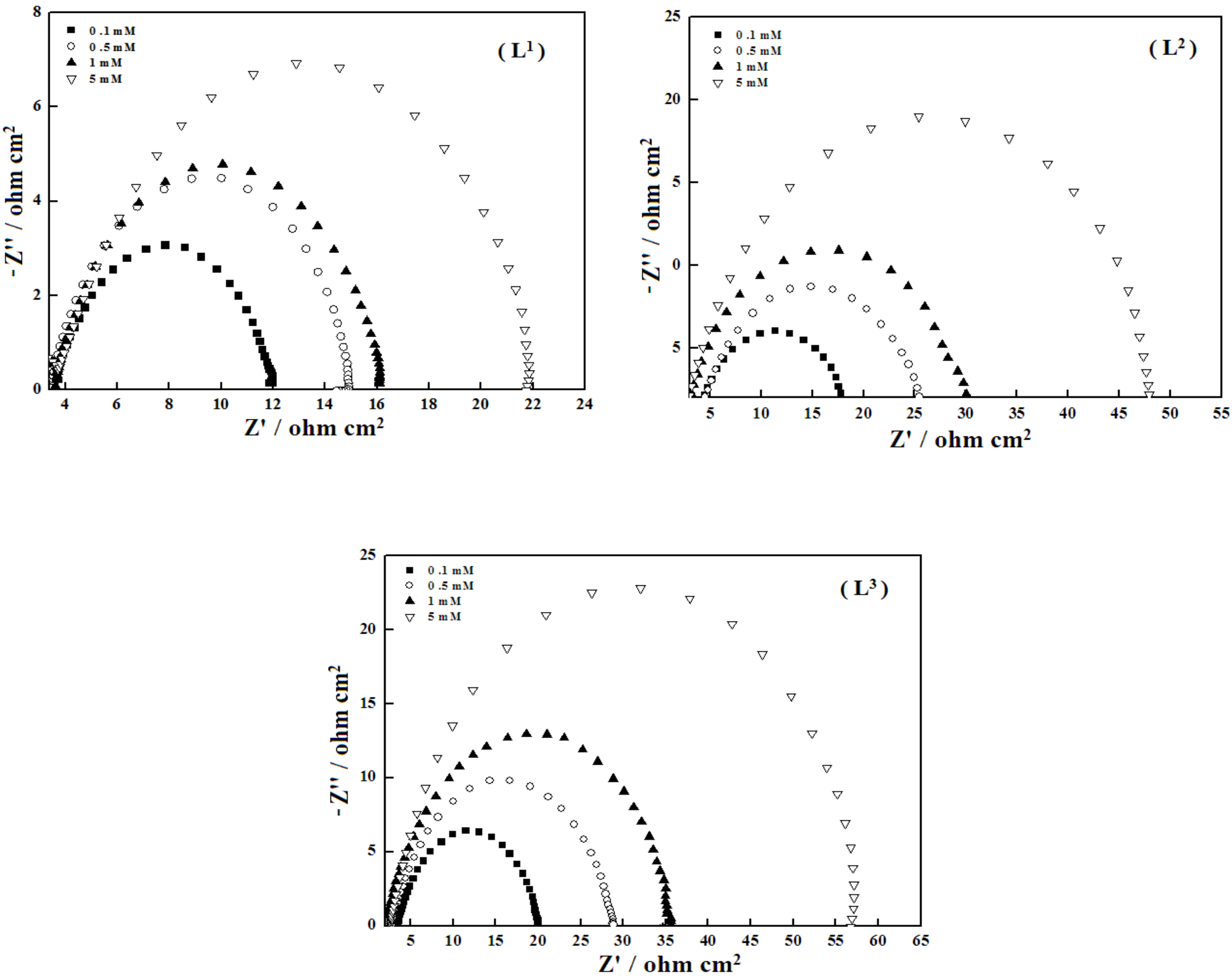

Fig. S8 Nyquist plots of mild steel in 1 M HCl containing different concentration of Schiff bases (L^1, L^2 and L^3).

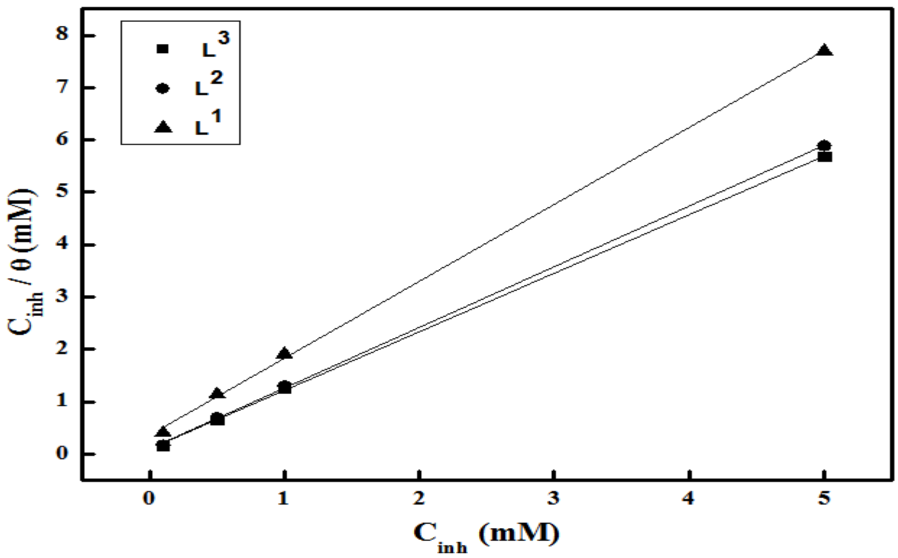

Fig. S9 Langmuir adsorption plots for mild steel in acidic media containing different concentration of Schiff bases.

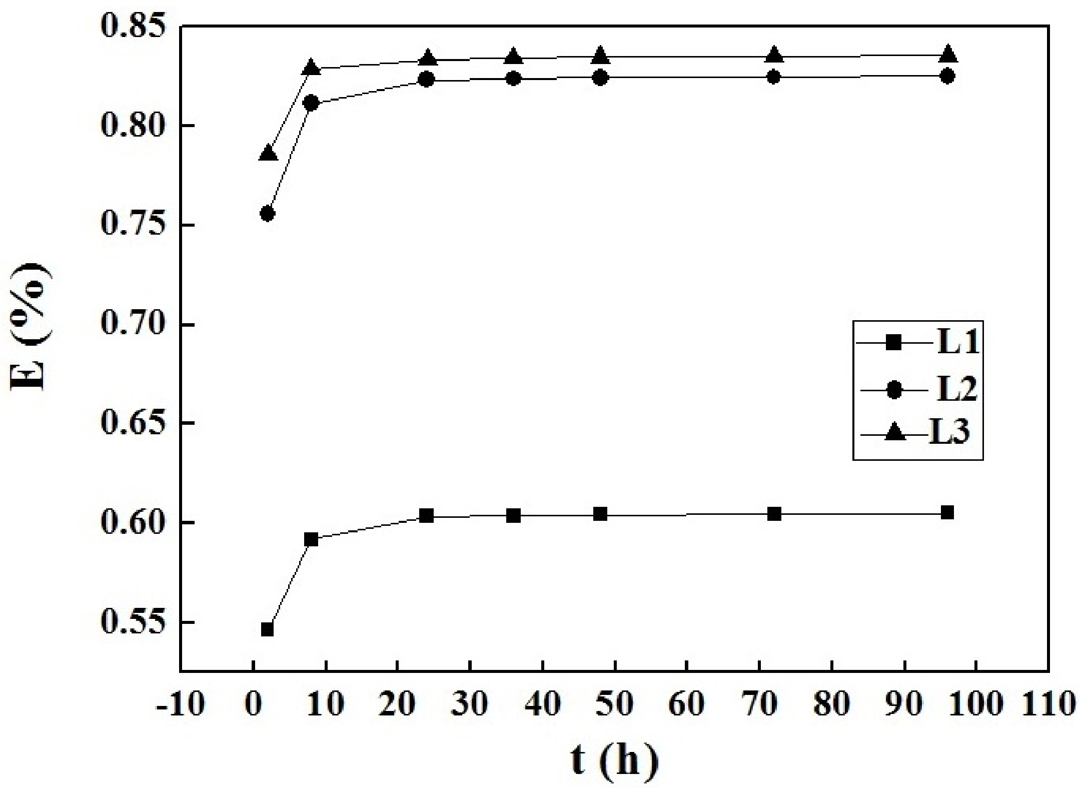

Fig. S10 Variation of inhibition efficiency obtained from weight loss measurement at 5 mM concentration of three Schiff bases having different immersion time (1-96 hr) towards corrosion of mild steel in 1M HCl.

Table S1 Calculated Fukui functions for the three inhibitor molecules

Atoms	L^1			L^2			L^3		
	f_k^+	f_k^-	f_k^0	f_k^+	f_k^-	f_k^0	f_k^+	f_k^-	f_k^0
O (1)	0.047	0.055	0.051	0.046	0.058	0.052	0.051	0.027	0.039
C (2)	0.046	0.038	0.042	0.045	0.041	0.043	0.052	0.019	0.036
C (3)	0.028	0.064	0.046	0.029	0.059	0.044	0.009	0.078	0.044
C (4)	0.021	0.061	0.041	0.021	0.056	0.039	0.006	0.073	0.040
N (5)	0.085	0.038	0.062	0.084	0.035	0.060	0.020	0.028	0.024
C (6)	0.120	0.040	0.080	0.115	0.038	0.077	0.013	0.047	0.030
C (7)	0.036	0.035	0.036	0.037	0.033	0.035	0.029	0.018	0.024
C (8)	0.041	0.028	0.035	0.042	0.031	0.037	0.037	0.015	0.026
C (9)	0.073	0.039	0.056	0.072	0.038	0.055	0.048	0.023	0.036
C (10)	0.038	0.043	0.041	0.029	0.036	0.033	0.032	0.016	0.024
C (11)	0.056	0.027	0.042	0.054	0.026	0.040	0.052	0.023	0.038
C (12)	0.037	0.036	0.037	0.037	0.033	0.036	0.008	0.041	0.025
C (13)	0.025	0.071	0.048	0.025	0.066	0.046	0.008	0.093	0.051
C (14)	0.045	0.062	0.054	0.045	0.056	0.051	0.011	0.066	0.039
C (15)	0.027	0.042	0.035	0.026	0.039	0.033	0.007	0.054	0.031
O (16)	0.026	0.084	0.055	0.026	0.078	0.052	0.010	0.109	0.060
Cl (17)	—	—	—	0.045	0.066	0.056	—	—	—
N (17)	—	—	—	—	—	—	0.125	0.010	0.068
O (18)	—	—	—	—	—	—	0.180	0.020	0.100
O (19)	—	—	—	—	—	—	0.181	0.022	0.102