

## **:Supplementary File:**

**Introduction of newly synthesized Schiff base molecules as efficient corrosion inhibitors for mild steel in 1 M HCl medium: an experimental, density functional theory and molecular dynamics simulation study**

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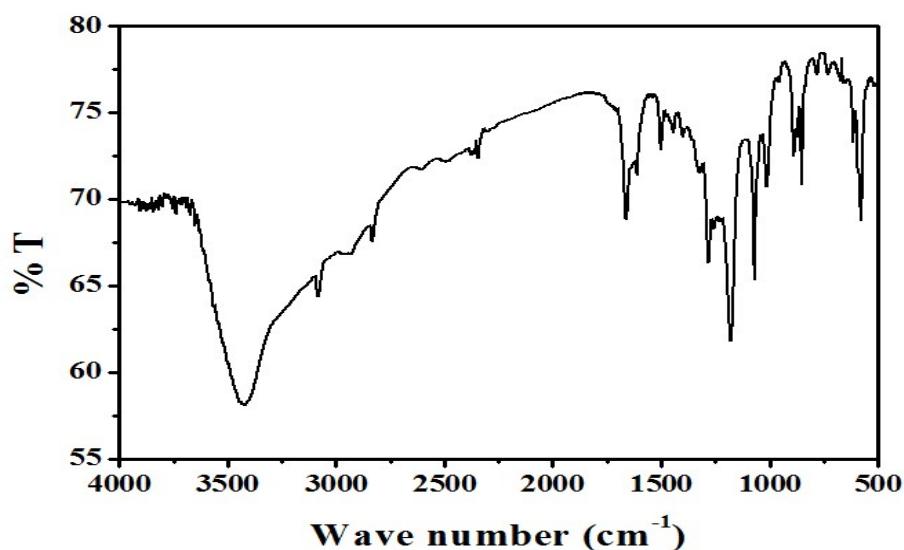


Fig. S1 FTIR spectrum of  $L^1$ .

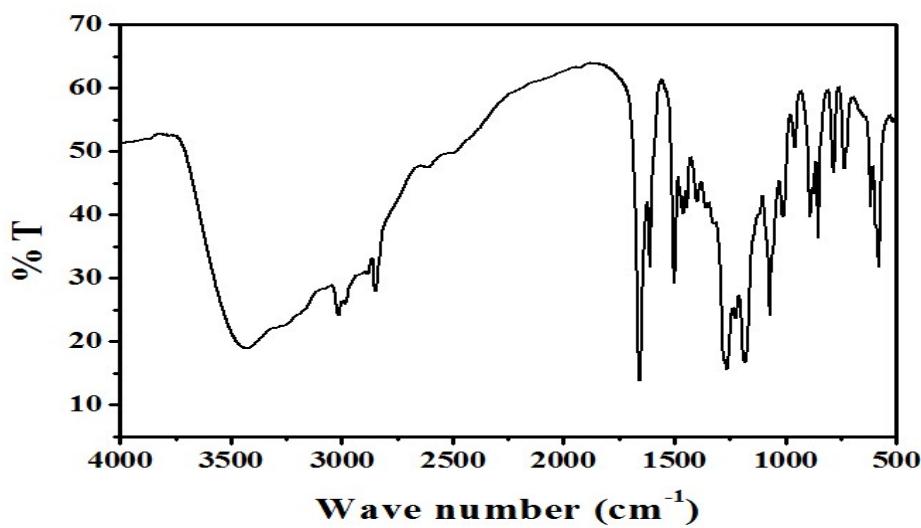


Fig. S2 FTIR spectrum of  $L^2$ .

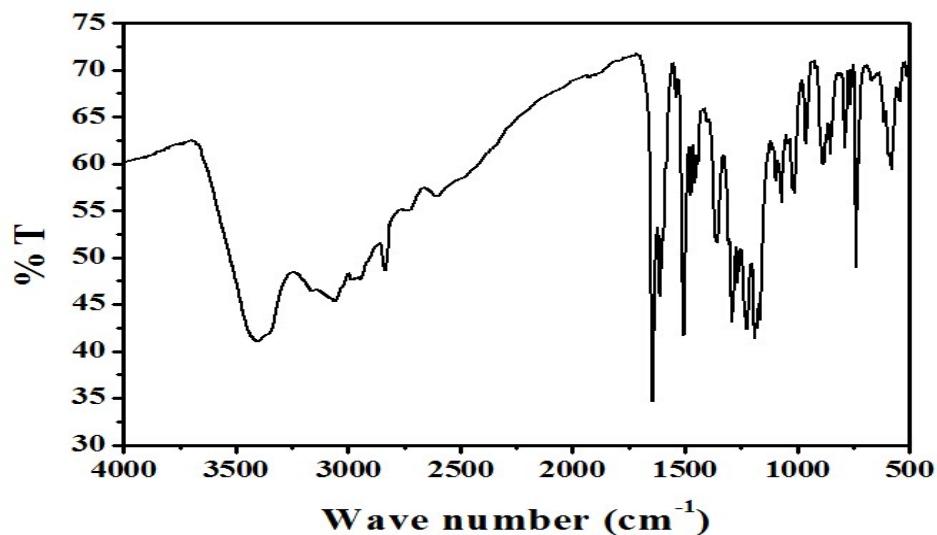
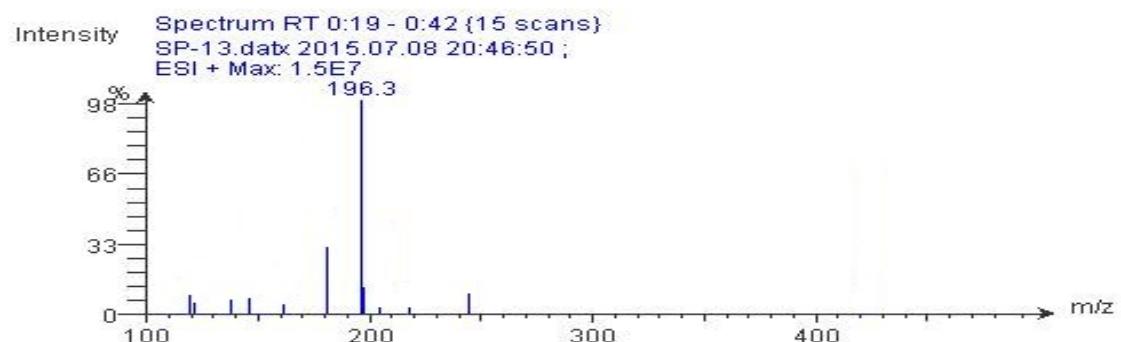
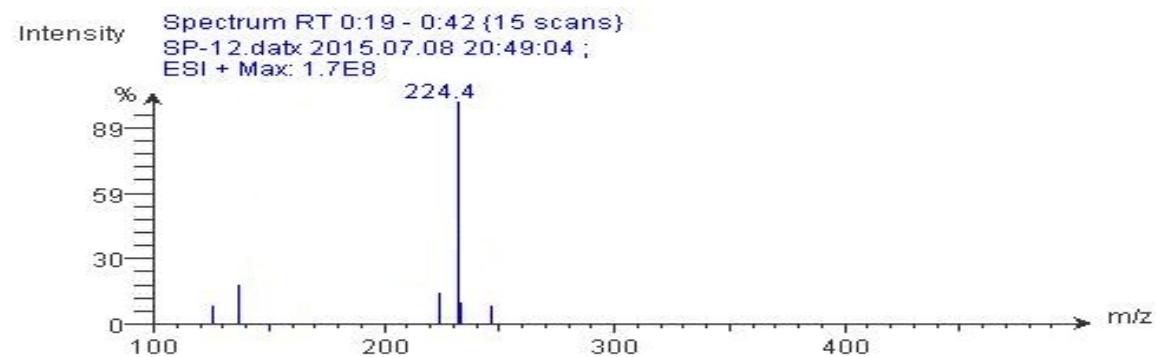


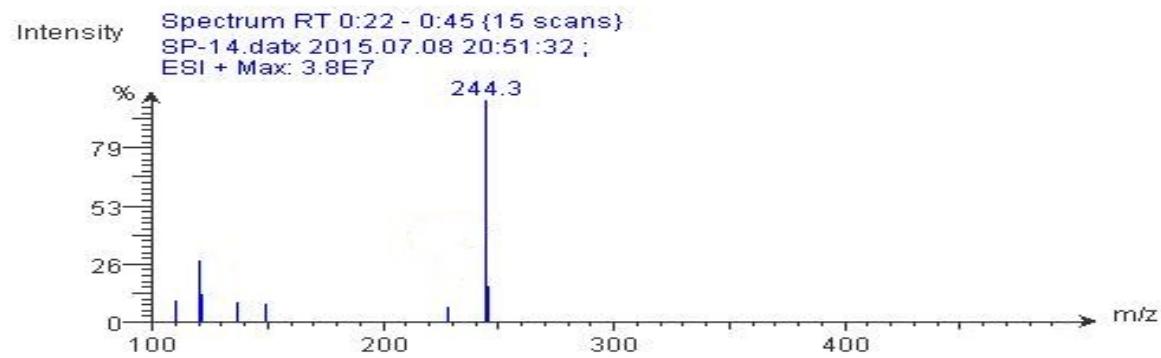
Fig. S3 FTIR spectrum of  $L^3$ .



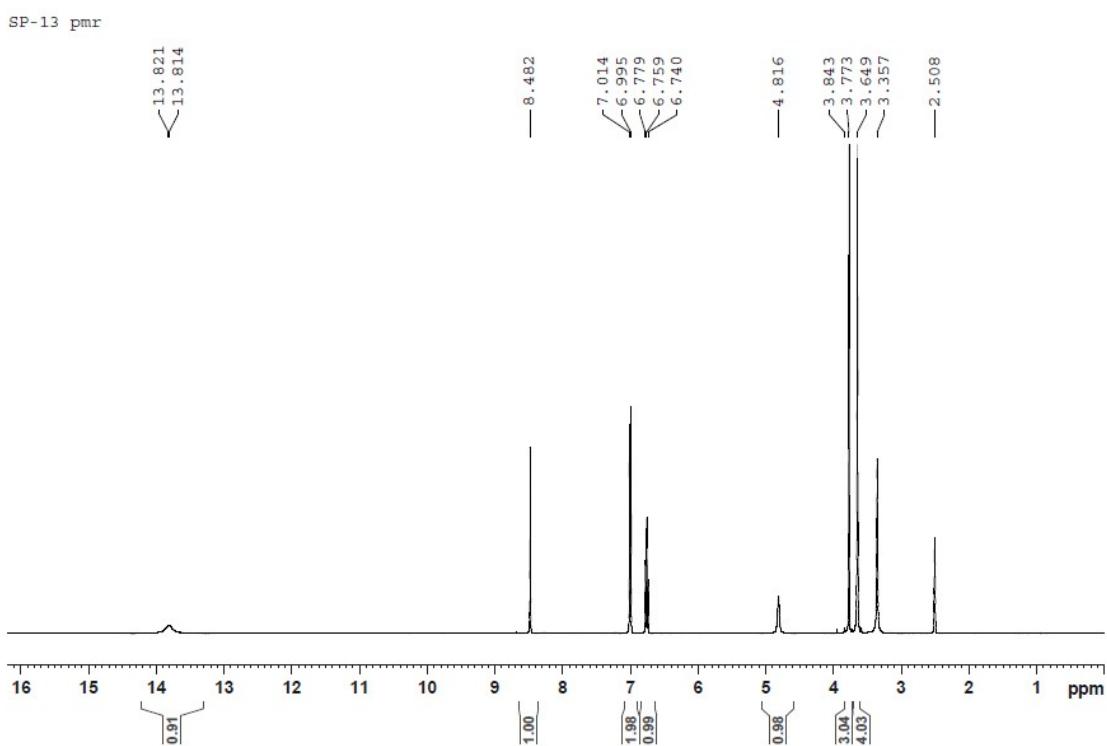
**Fig. S4** ESI-MS spectrum of L<sup>1</sup> in methanol.



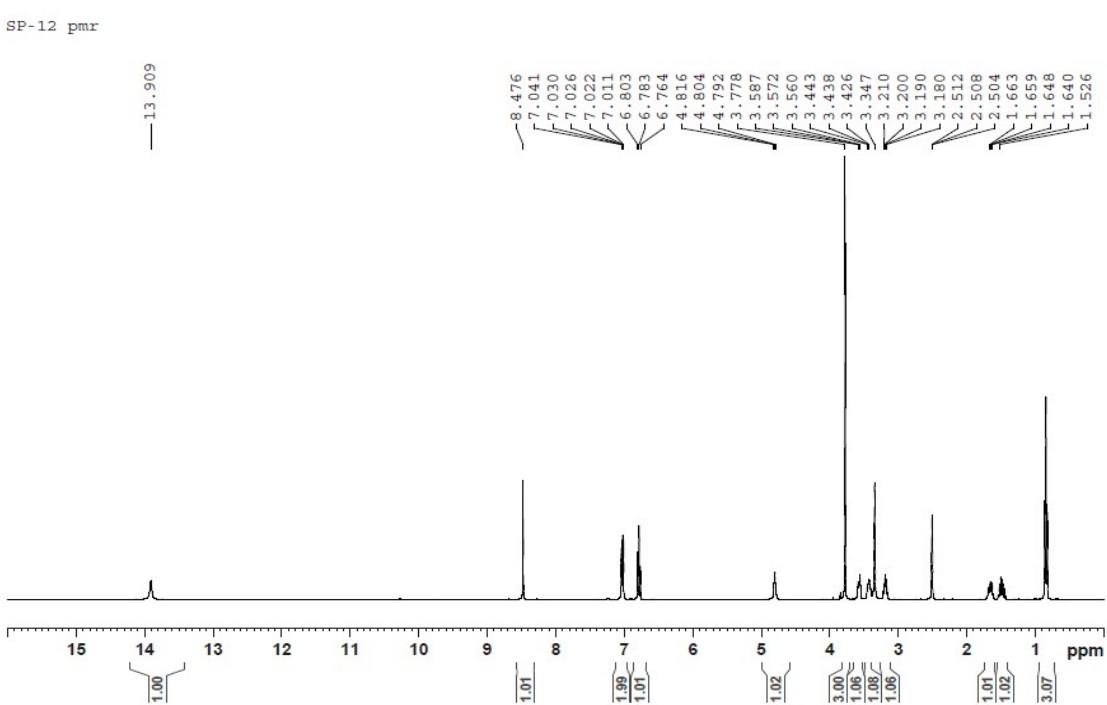
**Fig. S5** ESI-MS spectrum of L<sup>2</sup> in methanol.



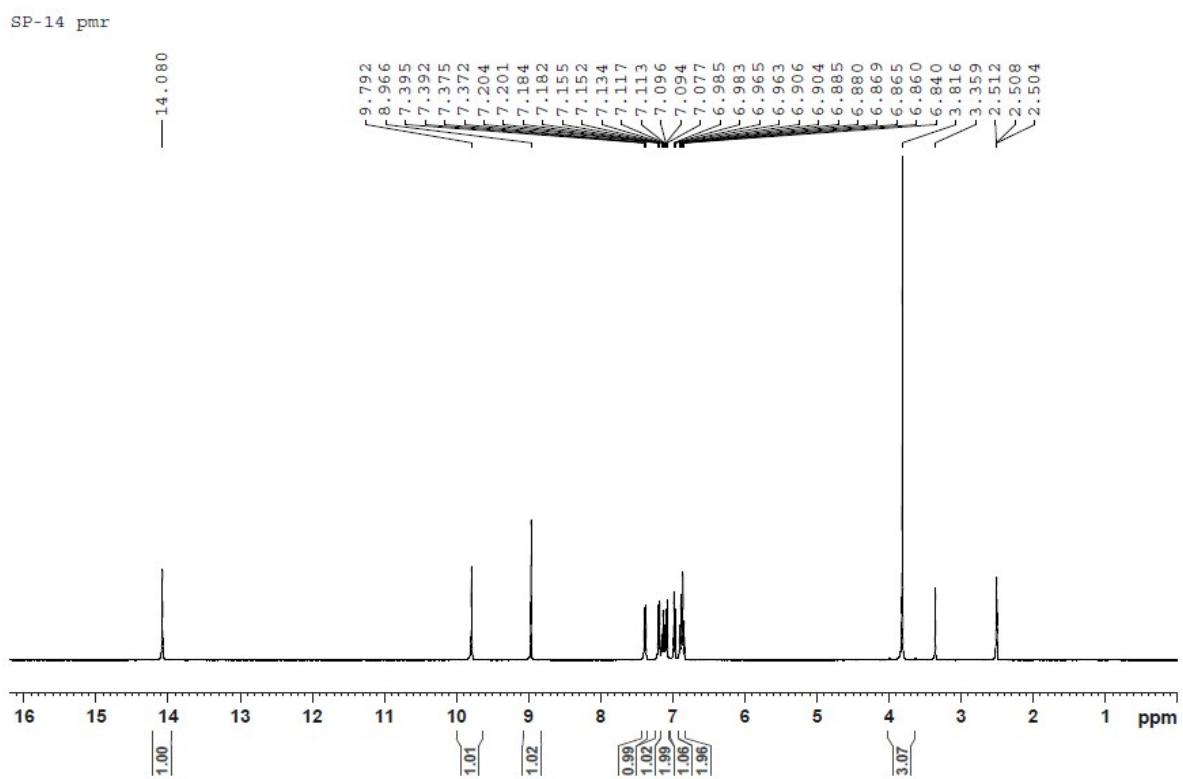
**Fig. S6** ESI-MS spectrum of L<sup>3</sup> in methanol.



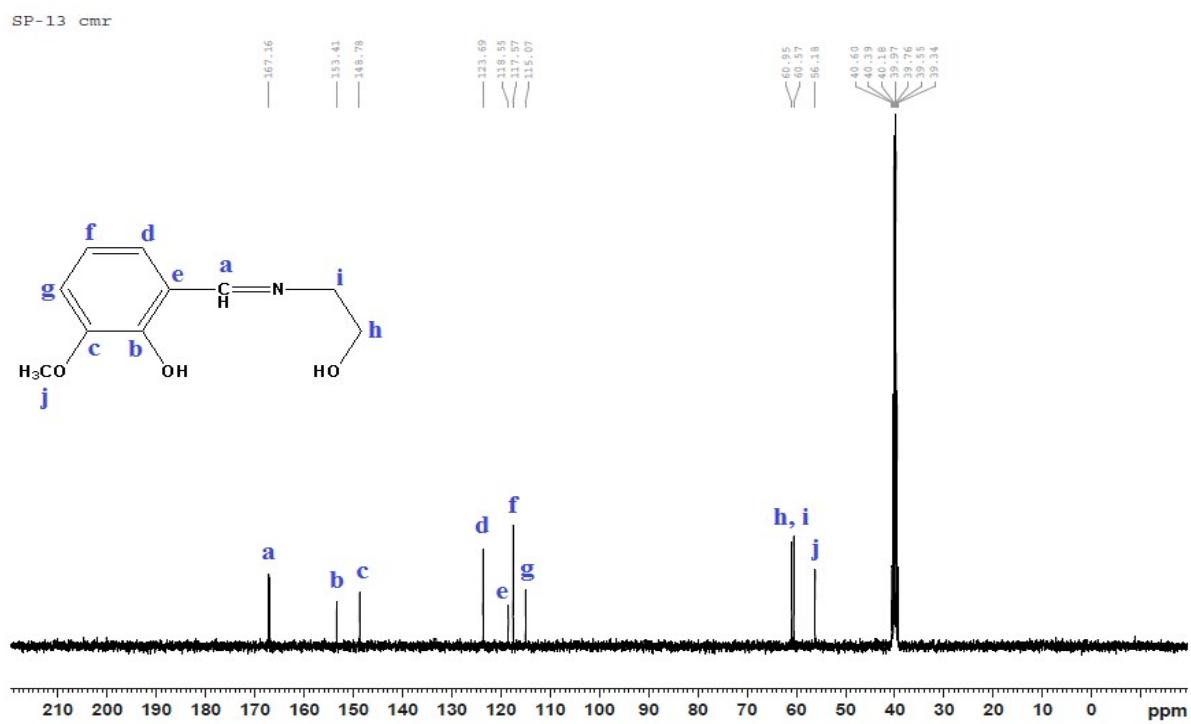
**Fig. S7**  $^1\text{H}$ -NMR of L<sup>1</sup> in DMSO-d<sub>6</sub>.



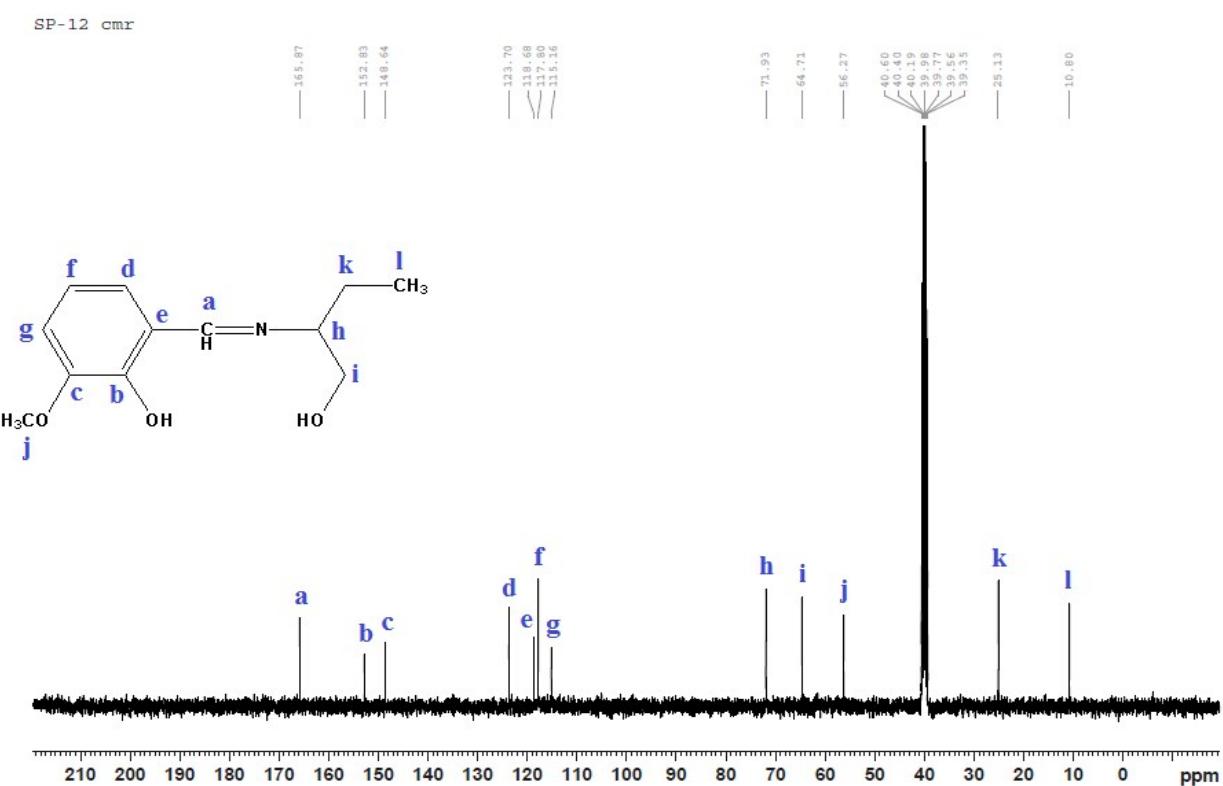
**Fig. S8**  $^1\text{H}$ -NMR of L<sup>2</sup> in DMSO-d<sub>6</sub>.



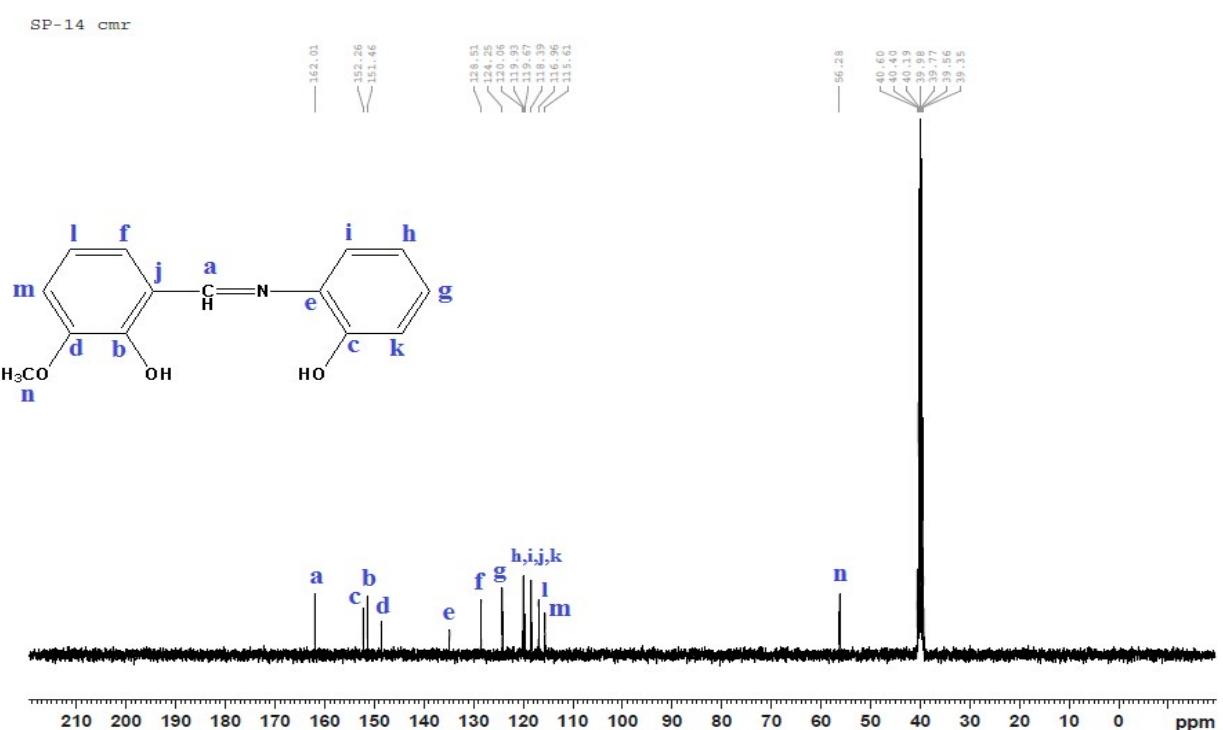
**Fig. S9**  $^1\text{H}$ -NMR of L<sup>3</sup> in DMSO-d<sub>6</sub>.



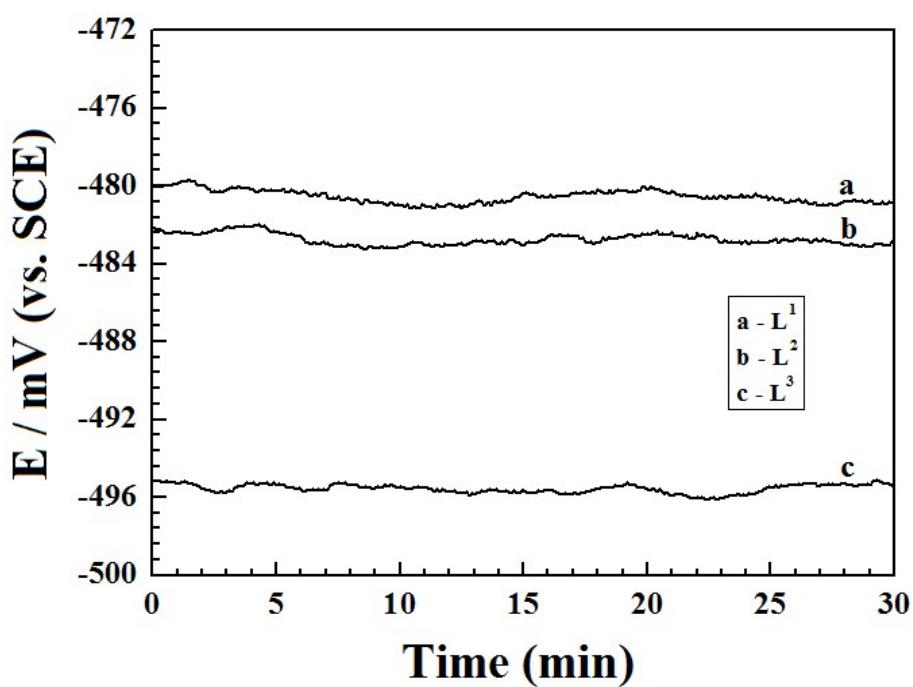
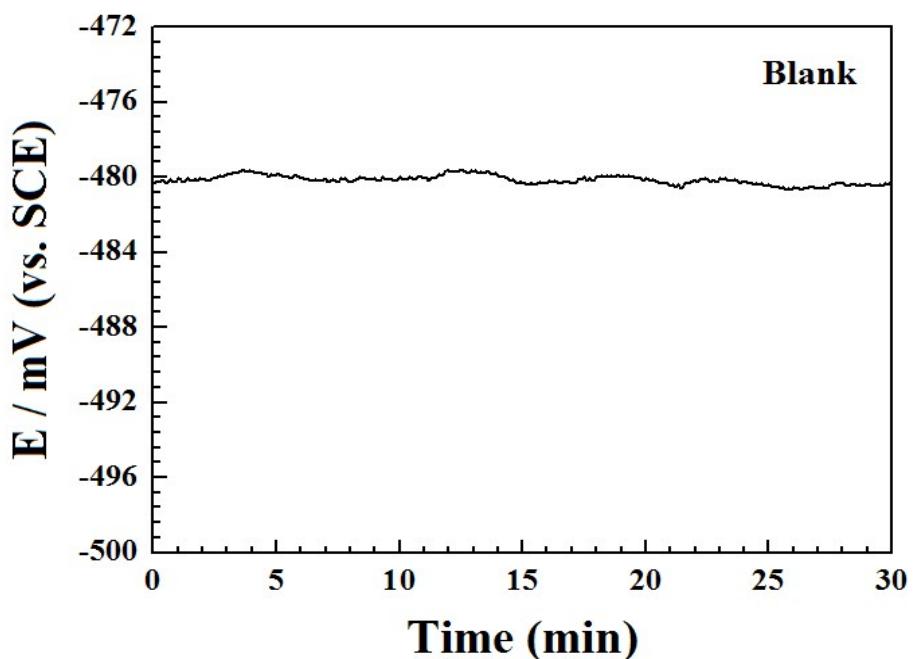
**Fig. S10**  $^{13}\text{C}$ -NMR of L<sup>1</sup> in DMSO-d<sub>6</sub>.



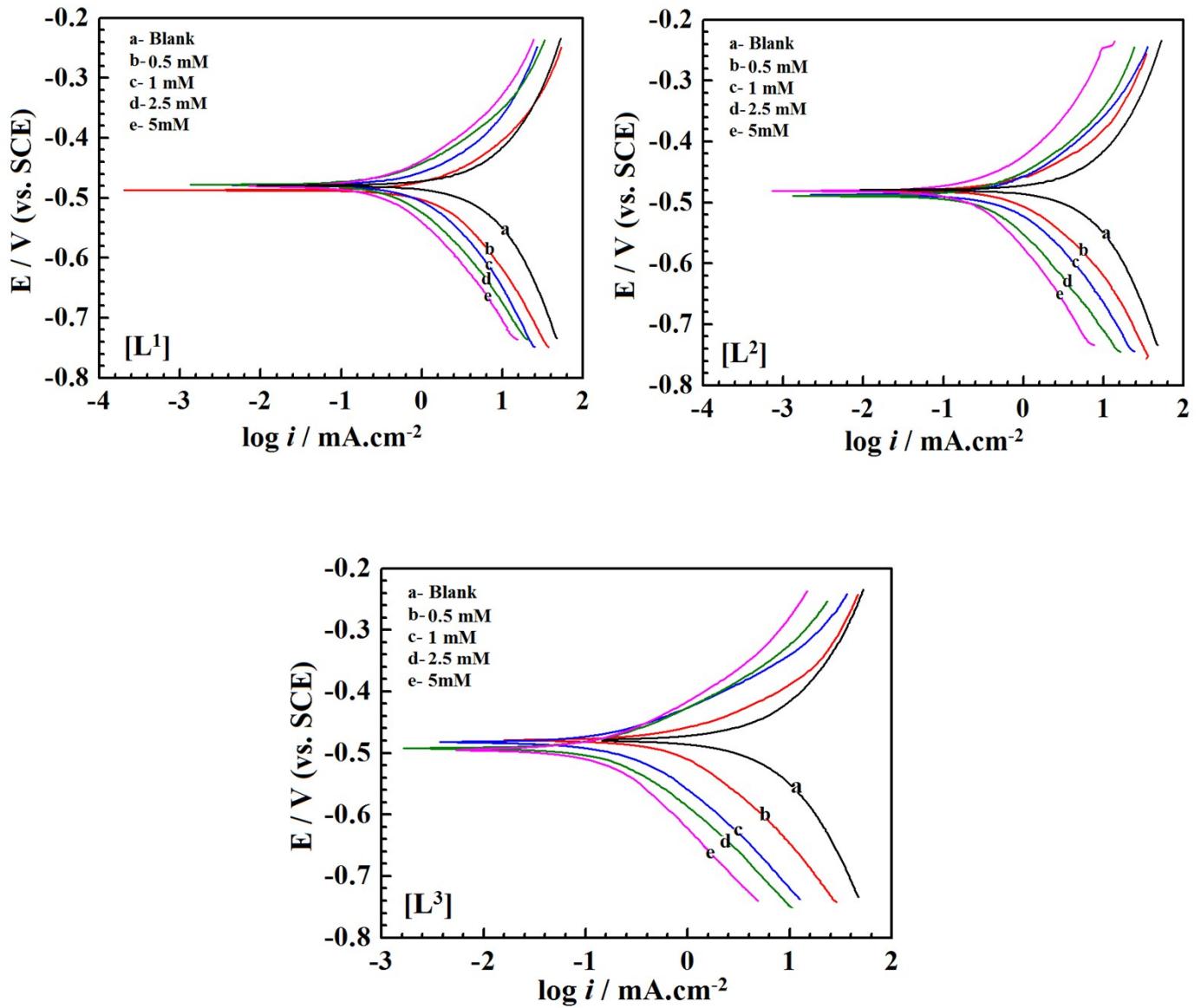
**Fig. S11**  $^{13}\text{C}$ -NMR of  $L^2$  in  $\text{DMSO-d}_6$ .



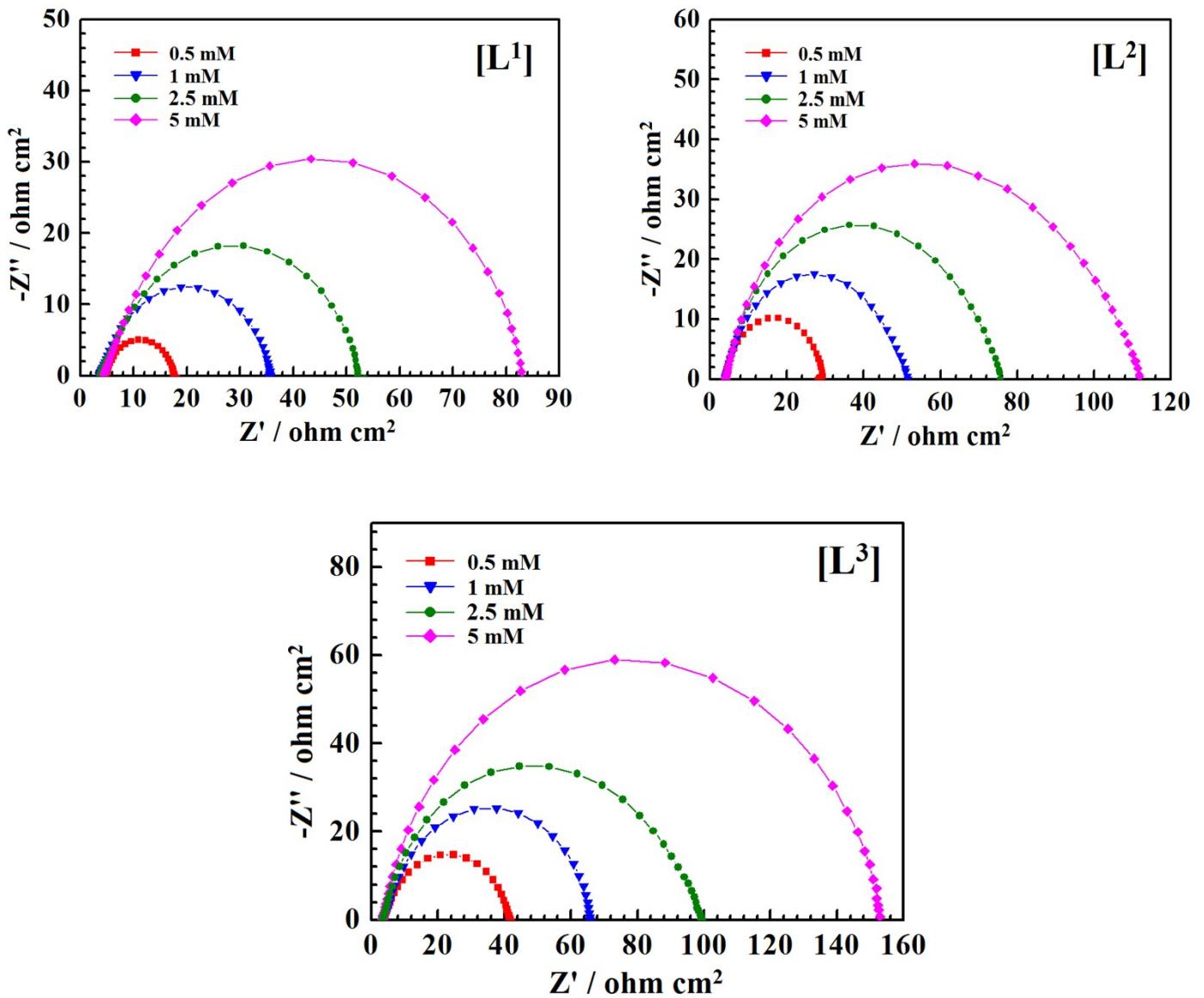
**Fig. S12**  $^{13}\text{C}$ -NMR of  $L^3$  in  $\text{DMSO-d}_6$ .



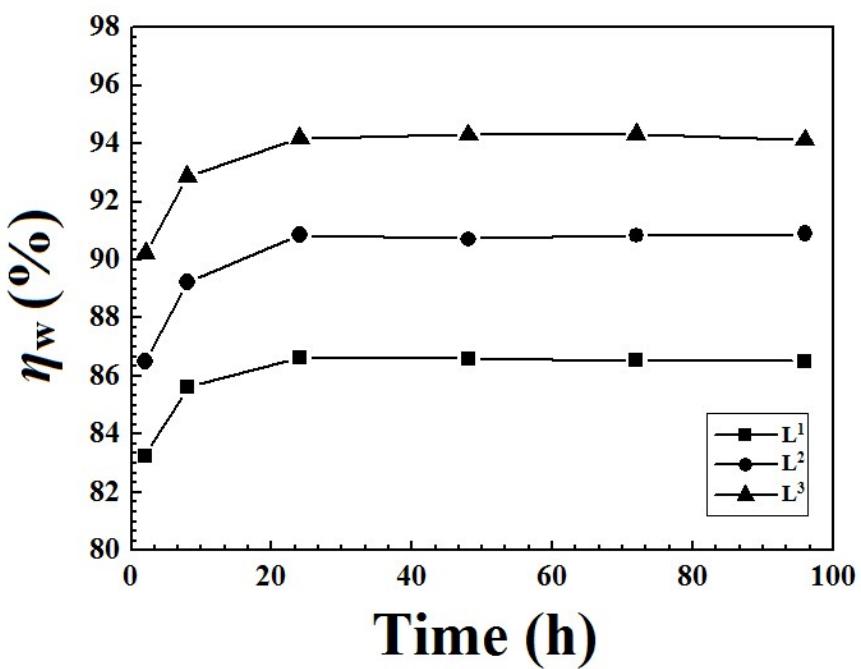
**Fig. 13** Variation of open circuit potential as a function of time for mild steel in 1 M HCl solution in the absence and presence of inhibitors at 5 mM concentration after exposure for 20 min.



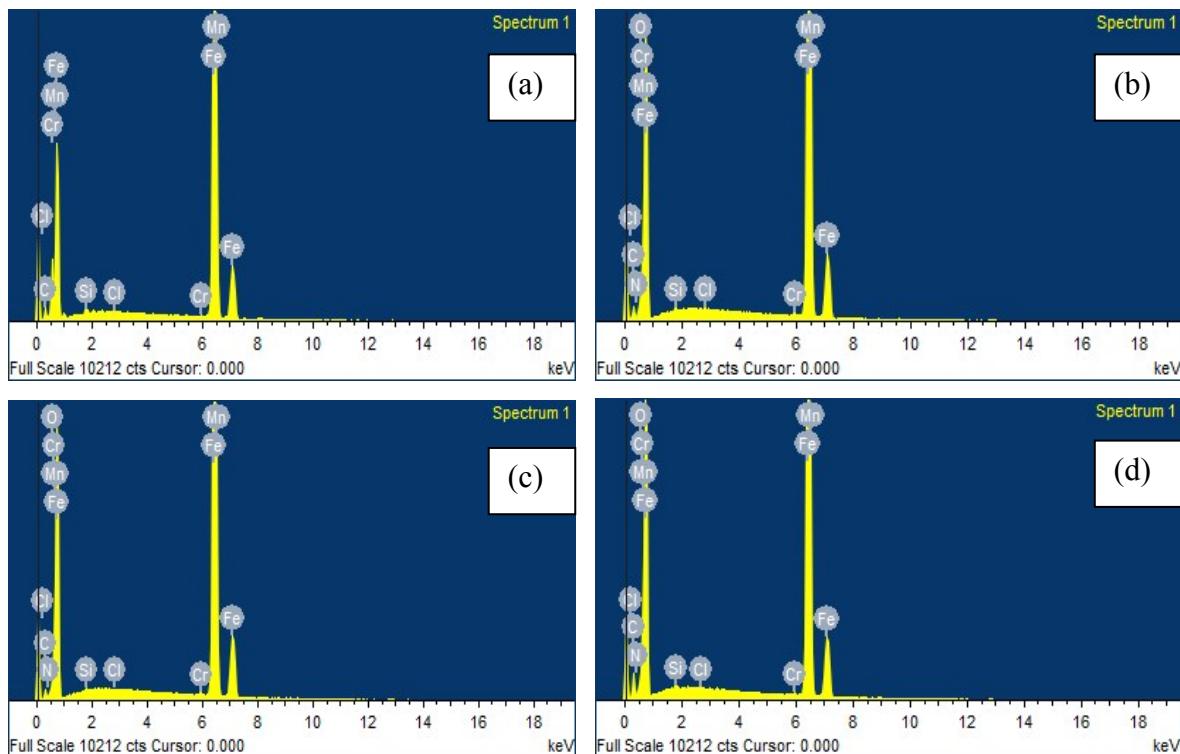
**Fig. S14** Potentiodynamics polarization curves of mild steel in 1 M HCl solution in the presence of different concentration of Schiff bases at 27°C.



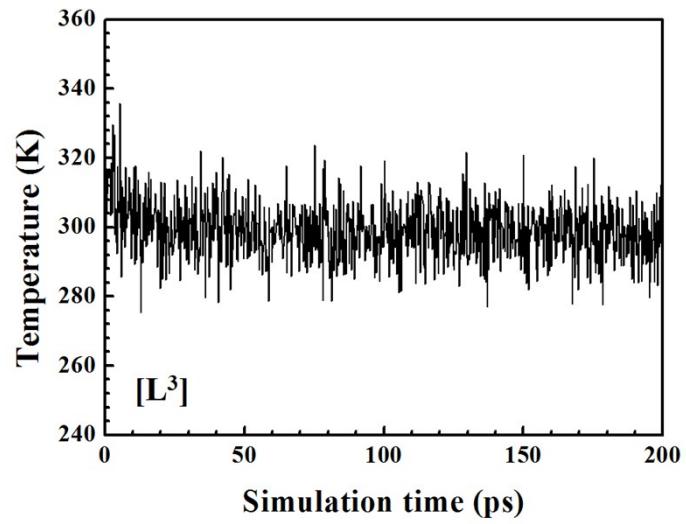
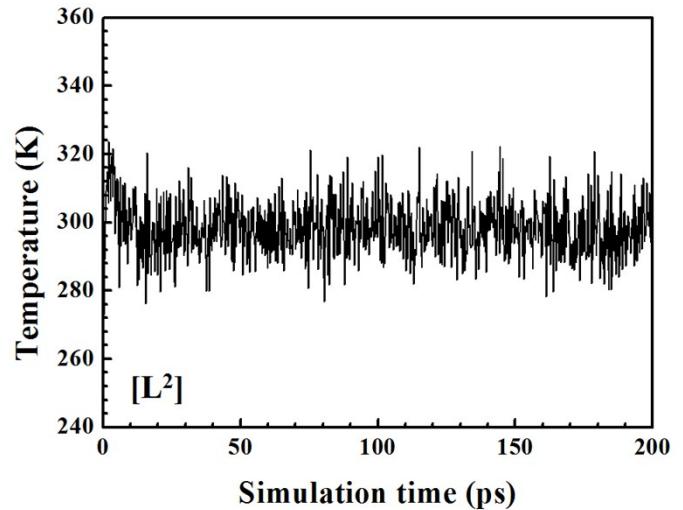
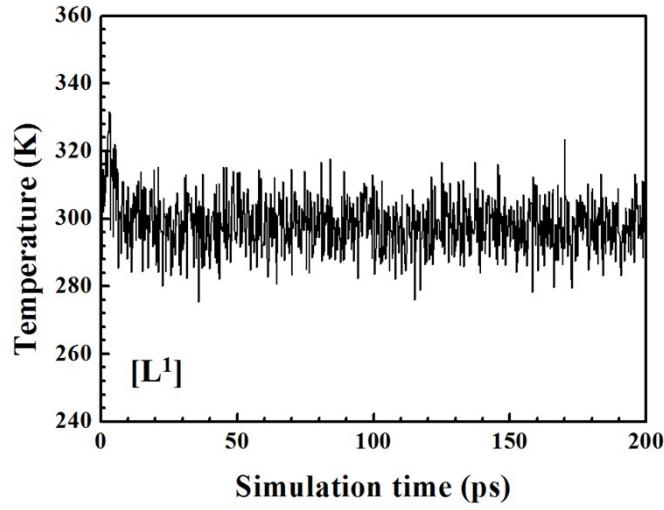
**Fig. S15** Nyquist plots of mild steel in 1 M HCl containing different concentration of Schiff bases ( $L^1$ ,  $L^2$  and  $L^3$ ) at 27°C.



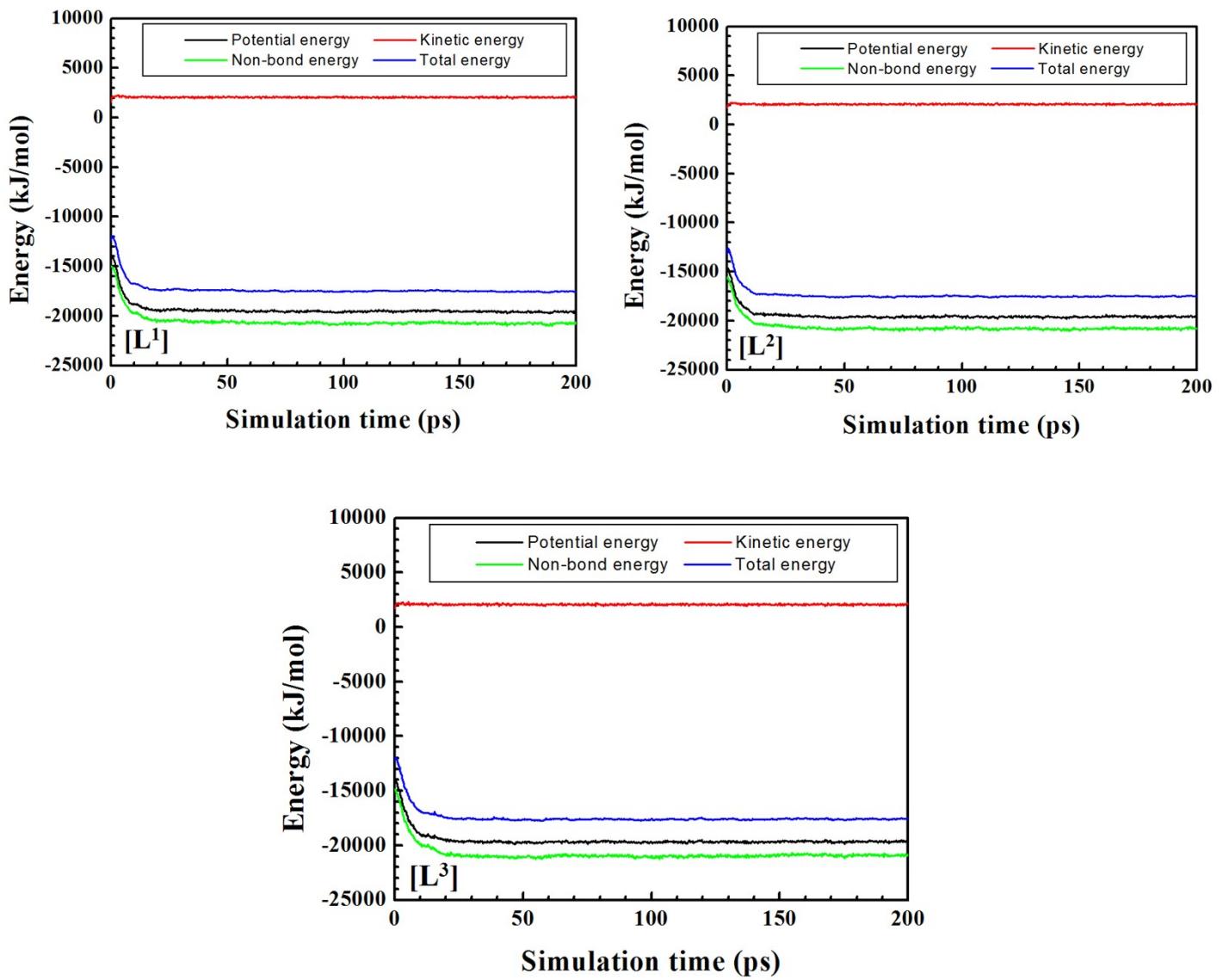
**Fig. S16** Variation of inhibition efficiency obtained from weight loss measurement at 5 mM concentration of three Schiff bases having different immersion time (2-96 h) towards corrosion of mild steel in 1 M HCl.



**Fig. S17** EDX spectra of mild steel surface obtained for (a) in absence of inhibitors and presence of (b)  $L^1$  (c)  $L^2$  and (d)  $L^3$  inhibitors.



**Fig. S18** Temperature equilibrium curve obtained from MD simulation for ( $L^1$ ), ( $L^2$ ) and ( $L^3$ ) at 300K.



**Fig. S19** Energy fluctuation curves obtained from MD simulation for ( $L^1$ ), ( $L^2$ ) and ( $L^3$ ) at 300 K.

**Equation S1**

$$E_{bond} = \sum_b [k_2(b - b_0)^2 + k_3(b - b_0)^3 + k_4(b - b_0)^4] \quad (1)$$

$$E_{angle} = \sum_{\theta} [H_2(\theta - \theta_0)^2 + H_3(\theta - \theta_0)^3 + H_4(\theta - \theta_0)^4] \quad (2)$$

$$E_{torsion} = \sum_{\phi} [V_1[1 - \cos(\phi - \phi_0)^2] + V_2[1 - \cos(2\phi - \phi_0)^2] + V_3[1 - \cos(3\phi - \phi_0)^2]] \quad (3)$$

$$E_{oop} = \sum_{\chi} k_{\chi} \chi^2 \quad (4)$$

$$\begin{aligned} E_{cross} = & \sum_b \sum_{b'} F_{bb'}(b - b_0)(b' - b_0) + \sum_{\theta} \sum_{\theta'} F_{\theta\theta'}(\theta - \theta_0)(\theta' - \theta_0) + \sum_b \sum_{\theta} F_{b\theta}(b - b_0)(\theta - \theta_0) \\ & + \sum_b \sum_{\phi} F_{b\phi}(b - b_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi] + \sum_{b'} \sum_{\phi} F_{b'\phi}(b' - b_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi] \\ & + \sum_{\theta} \sum_{\phi} F_{\theta\phi}(\theta - \theta_0)[V_1 \cos \phi + V_2 \cos 2\phi + V_3 \cos 3\phi] + \sum_{\theta} \sum_{\theta'} \sum_{\phi} k_{\phi\theta\theta'} \cos \phi (\theta - \theta_0)(\theta' - \theta_0) \end{aligned} \quad (5)$$

$$E_{elec} = \sum_{i,j} \frac{\mathbf{q}_i \mathbf{q}_j}{\epsilon r_{ij}} \quad (6)$$

$$E_{lj} = \sum_{i,j} \epsilon_{ij} \left[ 2 \left( \frac{r_{ij}^0}{r_{ij}} \right)^9 - 3 \left( \frac{r_{ij}^0}{r_{ij}} \right)^6 \right] \quad (7)$$

where  $b$  is the bond lengths,  $\theta$  refers to the valence angles,  $\phi$  is the torsion angles and  $\chi$  signifies out of plane angles, respectively.