Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Novel Schiff base molecules as efficient corrosion inhibitors for mild steel surface in 1 M HCl medium: Experimental and theoretical approach

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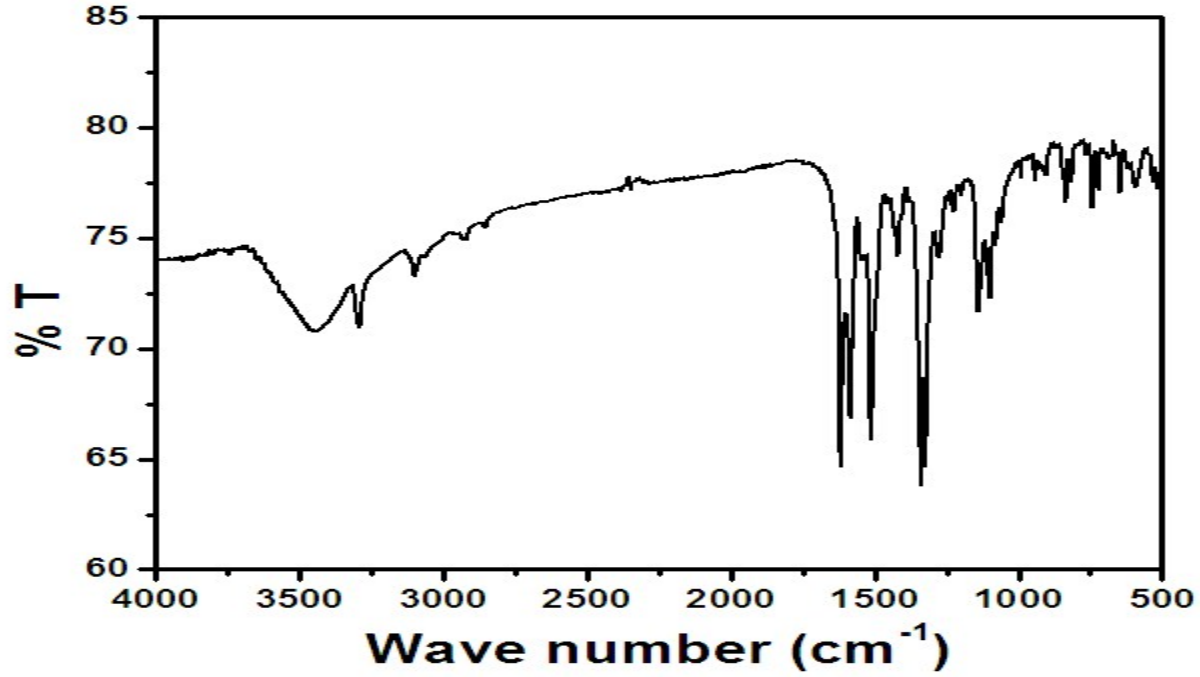


**Fig. S1** FTIR spectrum of $L^1$.

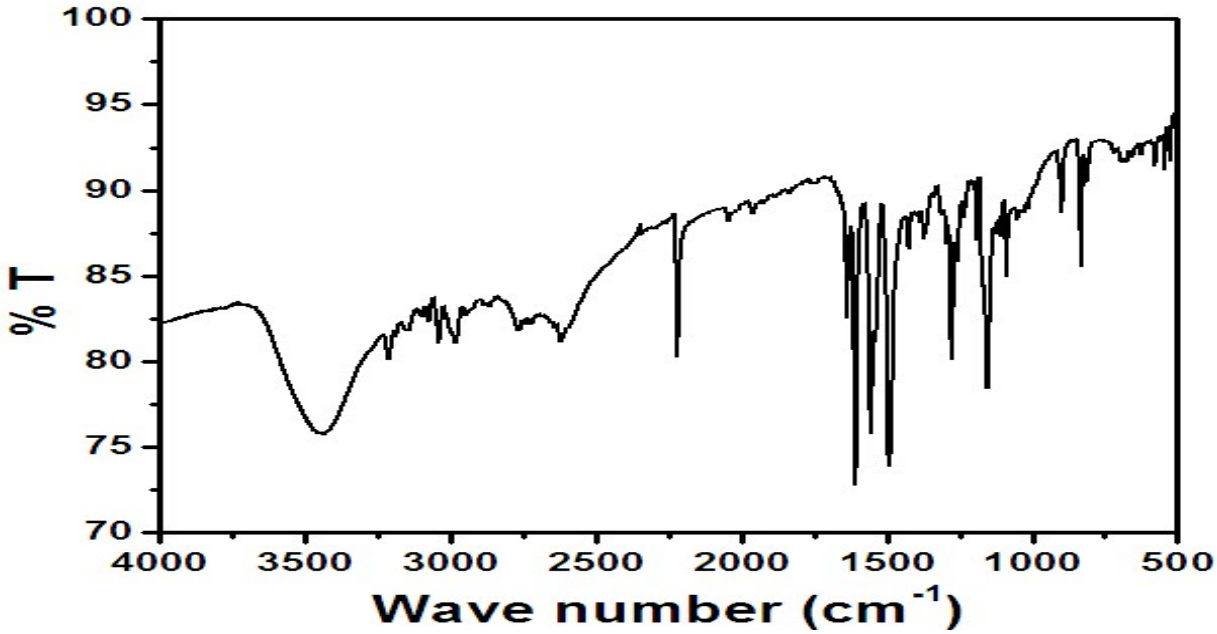


**Fig. S2** FTIR spectrum of $L^2$.

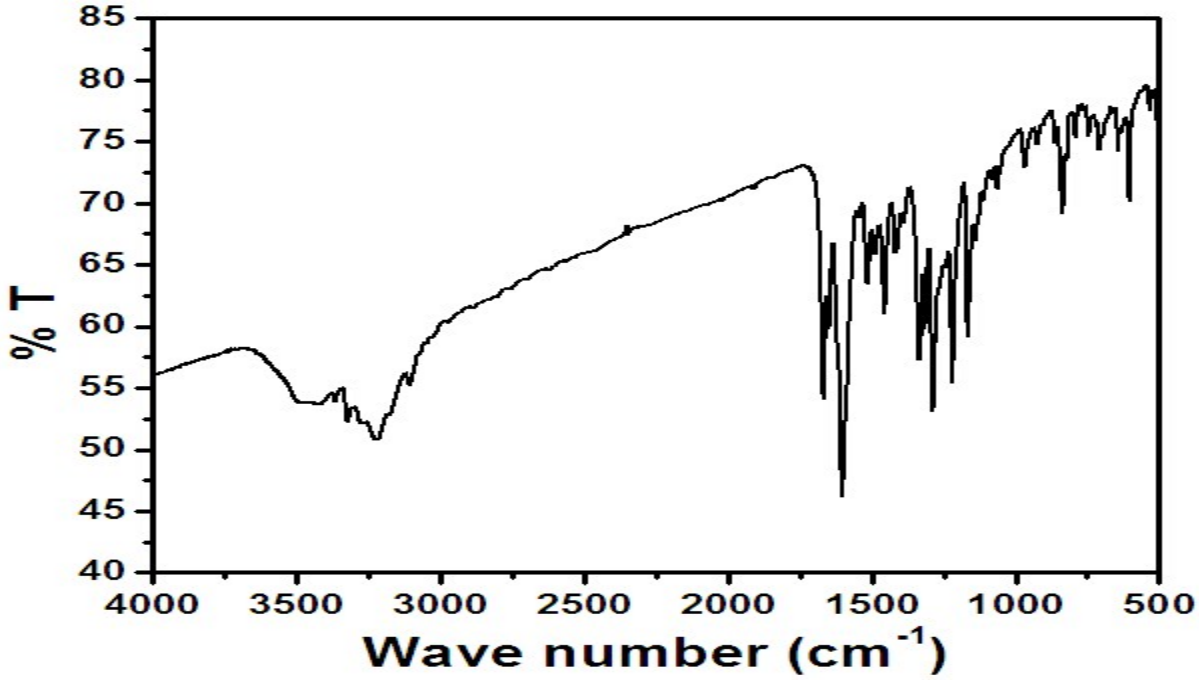


**Fig. S3** FTIR spectrum of $L^3$.

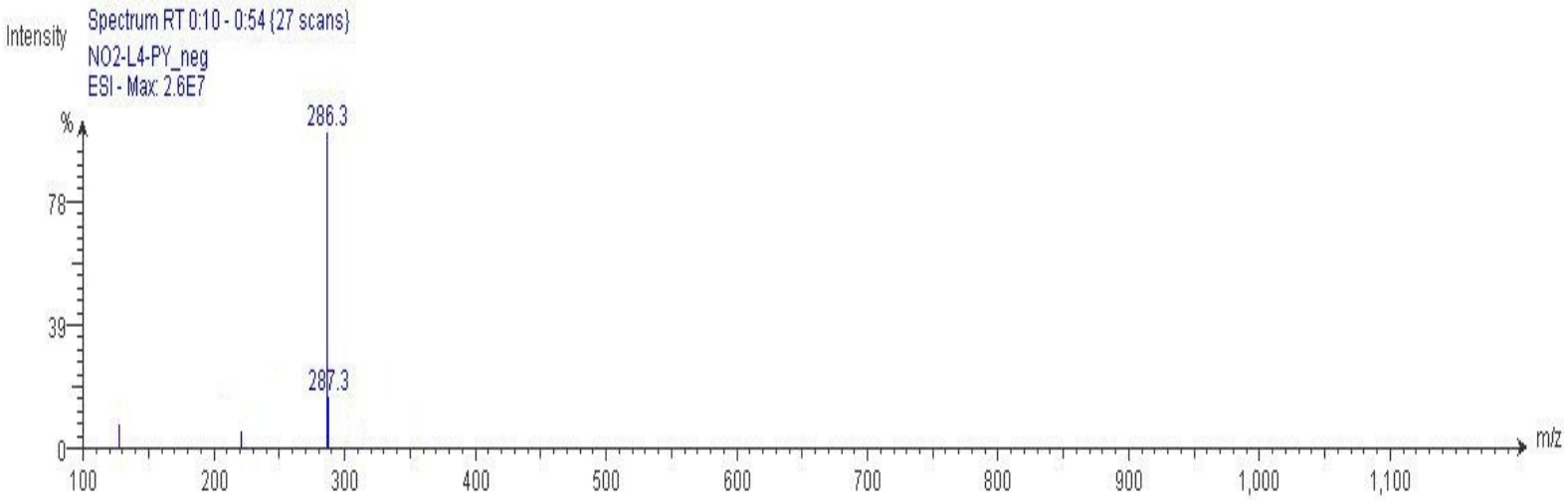


**Fig. S4** ESI-MS spectrum of $L^1$ in methanol.

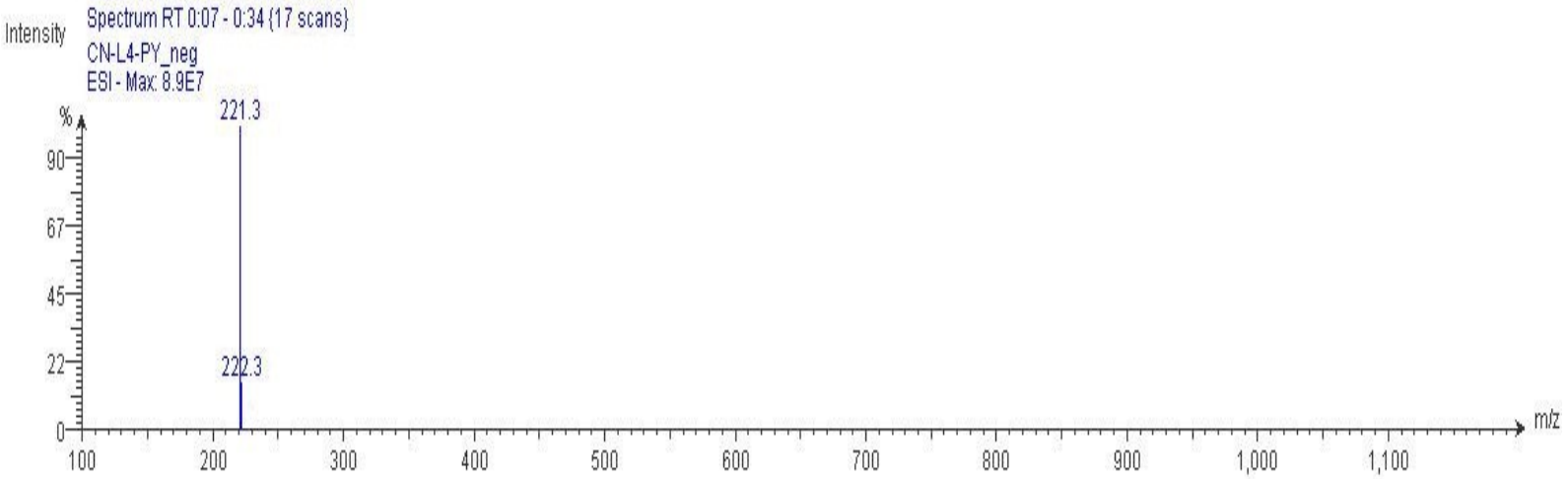


**Fig. S5** ESI-MS spectrum of $L^2$ in methanol.

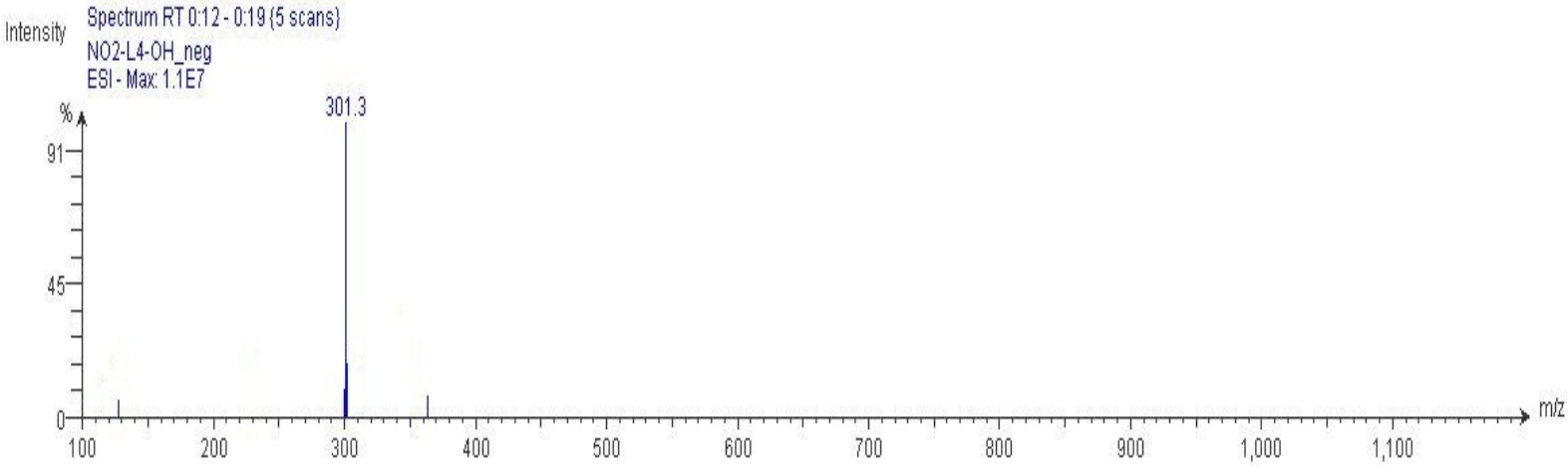


**Fig. S6** ESI-MS spectrum of $L^3$ in methanol.

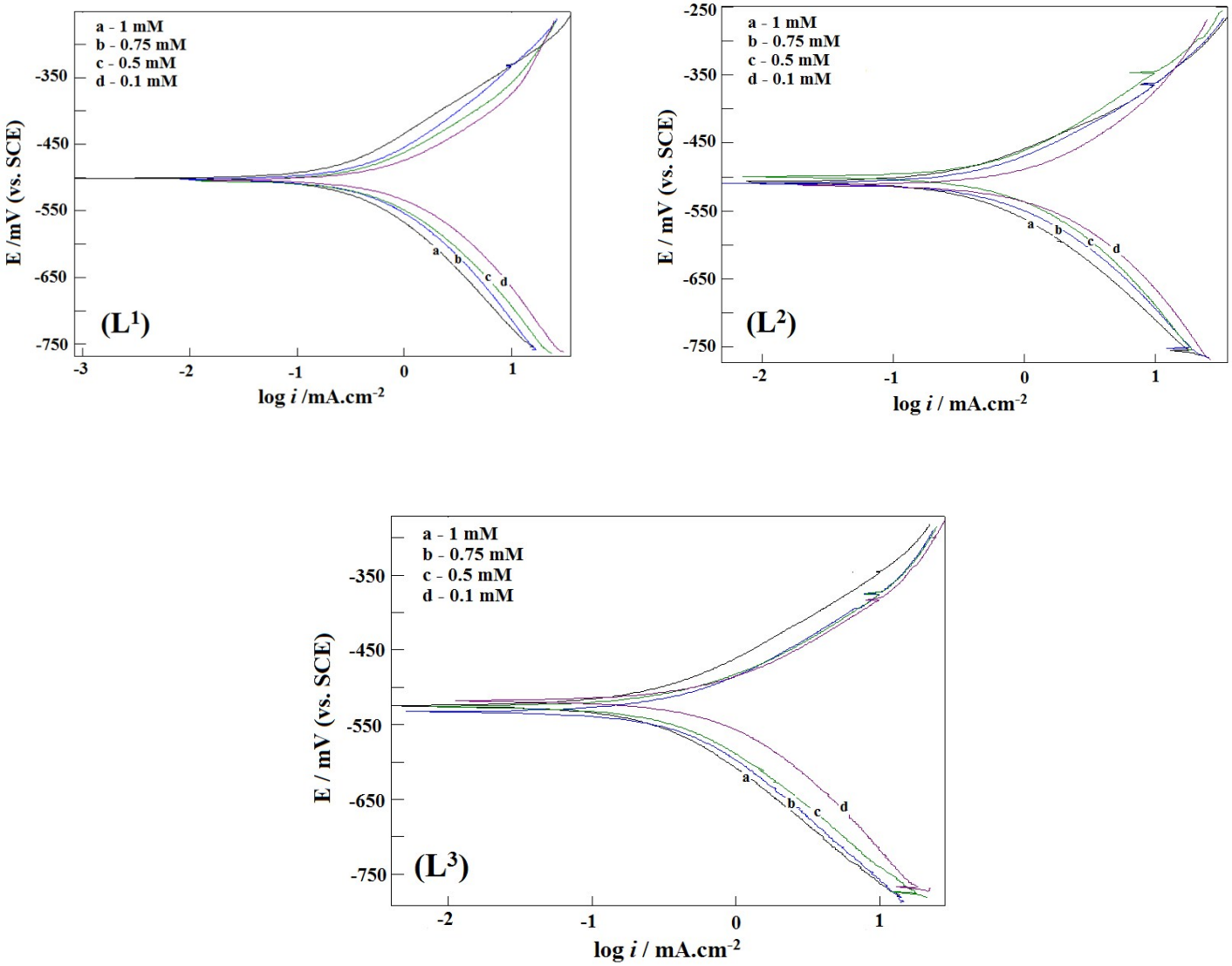


**Fig. S7** Tafel polarization curves for mild steel in 1 M HCl solution in the presence of Schiff bases ($L^1$, $L^2$ and $L^3$) with varying inhibitor concentration.

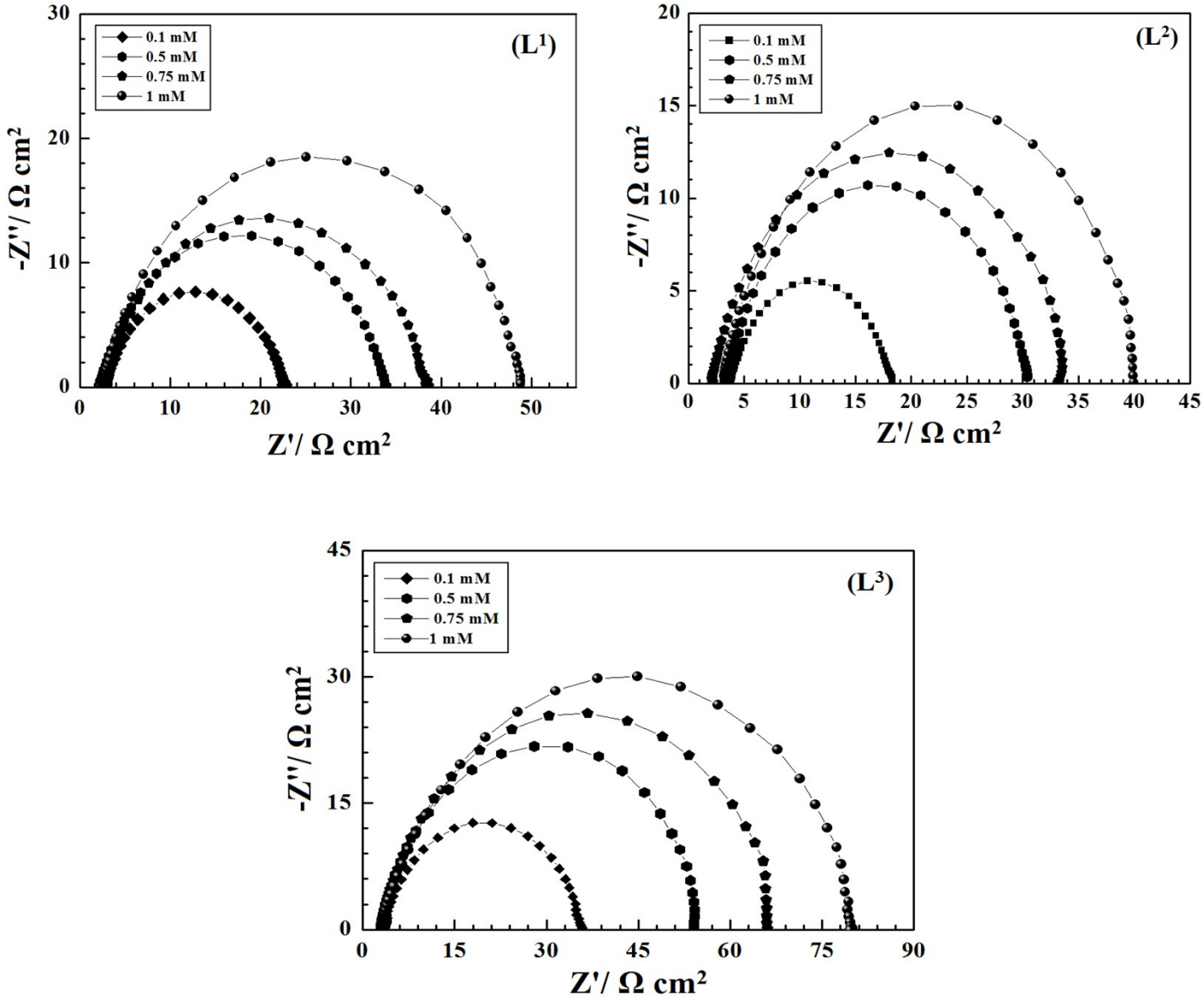


**Fig. S8** Nyquist impedance diagram for mild steel in 1 M HCl solution in presence of Schiff bases ($L^1$, $L^2$ and $L^3$) with different inhibitor concentration.

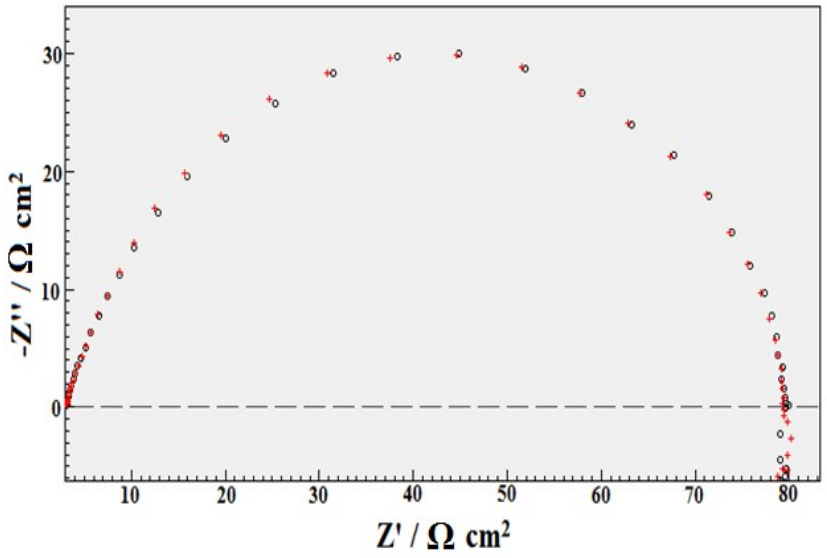


**Fig. S9** EIS fitting curve of $L^3$ inhibitor having 1mM concentration.

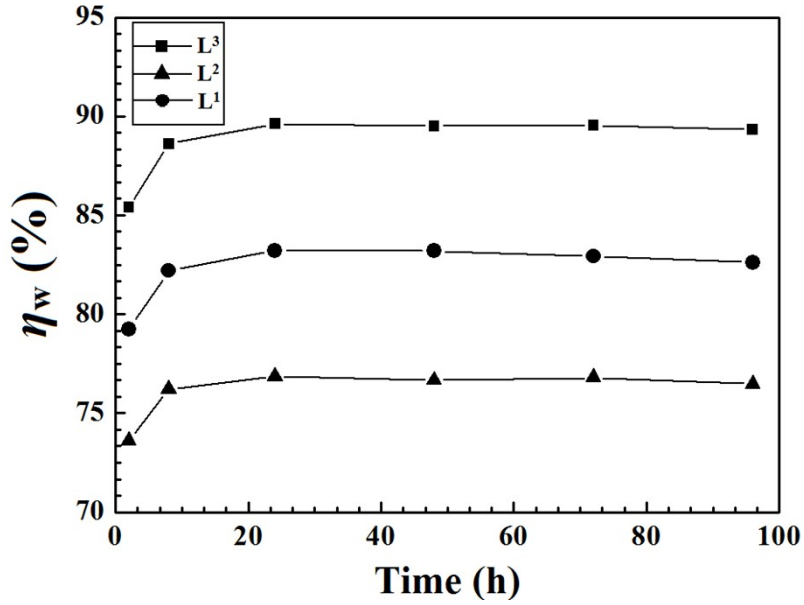


**Fig. S10** Variation of inhibition efficiency obtained from weight loss measurement at 1 mM concentration of three Schiff bases having different immersion time (1-96 hr) towards corrosion of mild steel in 1M HCl.

**Table S1** Calculated Fukui indices of the three Schiff base inhibitors

| Atoms | $L^1$ | | | $L^2$ | | | $L^3$ | | |
|---|---|---|---|---|---|---|---|---|---|
| | $f_k^+$ | $f_k^-$ | $f_k^0$ | $f_k^+$ | $f_k^-$ | $f_k^0$ | $f_k^+$ | $f_k^-$ | $f_k^0$ |
| N (1) | 0.016 | 0.058 | 0.037 | 0.078 | 0.044 | 0.061 | — | — | — |
| C (1) | — | — | — | — | — | — | 0.015 | 0.049 | 0.032 |
| C (2) | 0.033 | 0.067 | 0.050 | 0.085 | 0.087 | 0.086 | 0.026 | 0.040 | 0.033 |
| C (3) | 0.031 | 0.050 | 0.041 | 0.028 | 0.053 | 0.041 | 0.038 | 0.031 | 0.031 |
| C (4) | 0.029 | 0.047 | 0.038 | 0.033 | 0.062 | 0.048 | 0.031 | 0.029 | 0.030 |
| C (5) | 0.038 | 0.026 | 0.029 | 0.030 | 0.037 | 0.034 | 0.025 | 0.021 | 0.023 |
| C (6) | 0.009 | 0.024 | 0.017 | 0.042 | 0.022 | 0.032 | 0.010 | 0.041 | 0.024 |
| C (7) | 0.029 | 0.035 | 0.032 | 0.025 | 0.055 | 0.040 | 0.030 | 0.025 | 0.028 |
| C (8) | 0.007 | 0.023 | 0.015 | 0.054 | 0.019 | 0.037 | 0.011 | 0.051 | 0.031 |
| C (9) | 0.012 | 0.034 | 0.023 | 0.053 | 0.033 | 0.043 | 0.013 | 0.036 | 0.025 |
| C (10) | 0.009 | 0.025 | 0.017 | 0.050 | 0.022 | 0.036 | 0.011 | 0.042 | 0.027 |
| C (11) | 0.059 | 0.029 | 0.044 | 0.030 | 0.033 | 0.032 | 0.063 | 0.022 | 0.043 |
| C (12) | 0.012 | 0.034 | 0.023 | 0.048 | 0.034 | 0.041 | 0.013 | 0.036 | 0.025 |
| C (13) | 0.040 | 0.033 | 0.036 | 0.023 | 0.034 | 0.029 | 0.032 | 0.026 | 0.029 |
| N (14) | 0.014 | 0.050 | 0.032 | 0.094 | 0.046 | 0.070 | 0.016 | 0.060 | 0.038 |
| N (15) | 0.029 | 0.079 | 0.054 | 0.033 | 0.100 | 0.067 | 0.032 | 0.048 | 0.040 |
| N (16) | 0.048 | 0.021 | 0.035 | — | — | — | 0.049 | 0.020 | 0.035 |
| C (16) | — | — | — | 0.029 | 0.034 | 0.032 | — | — | — |
| O (17) | 0.080 | 0.043 | 0.062 | — | — | — | 0.082 | 0.039 | 0.060 |
| N (17) | — | — | — | 0.050 | 0.072 | 0.061 | — | — | — |
| O (18) | 0.075 | 0.045 | 0.060 | — | — | — | 0.077 | 0.039 | 0.058 |
| N (19) | 0.083 | 0.022 | 0.053 | — | — | — | 0.076 | 0.025 | 0.051 |
| O (20) | 0.123 | 0.049 | 0.086 | — | — | — | 0.113 | 0.048 | 0.081 |
| O (21) | 0.117 | 0.040 | 0.078 | — | — | — | 0.108 | 0.039 | 0.074 |
| O (22) | — | — | — | — | — | — | 0.016 | 0.062 | 0.039 |