Investigating the Effectiveness of an Imidazopyridine-Based Compound as an Anti-corrosive Additive for Mild Steel in Molar Hydrochloric Solutions: A Mutual Multi-Facet Experimental and Computational Approach

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NMR ^{1}H, NMR ^{13}C and IR data of MPPIP

NMR **^{1}H** (300 MHz, DMSO, δ ppm): 8.659 (s, 1H, HC_{18}=N); 8.322 (d, 1H, C_3H, J= 6.99Hz); 7.842 (d, 2H, $C_{12}H$ $C_{16}H$, J=7.29Hz); 7.654 (d,2H, $C_{15}H$ + $C_{13}H$, J=22,2Hz); 7.35 (q, 4H, C_6H + $C_{14}H$, $C_{24}H$ + $C_{20}H$); 6.75 (d, 3H, C_2H + $C_{23}H$ + $C_{21}H$, J =6.09Hz); 2.41 (s, 3H, $C_{17}H$).

NMR **^{13}C** (75 MHz, DMSO, δ ppm): 171.94; 160.87; 158.06; 142.28; 135.41; 134.78; 132.47; 130.38; 128.55; 128.48; 127.54; 127.26; 123.04; 115.80; 115.22; 115.02; 20.76.

m/z (M+): 328.00.

IR: ν (O-H) = 3477 cm^{-1}; ν (CH=N, imine) = 1659 cm^{-1}; ν(C=C) = 1585cm^{-1}; ν(C-O) = 1186 and 1156 cm^{-1}.

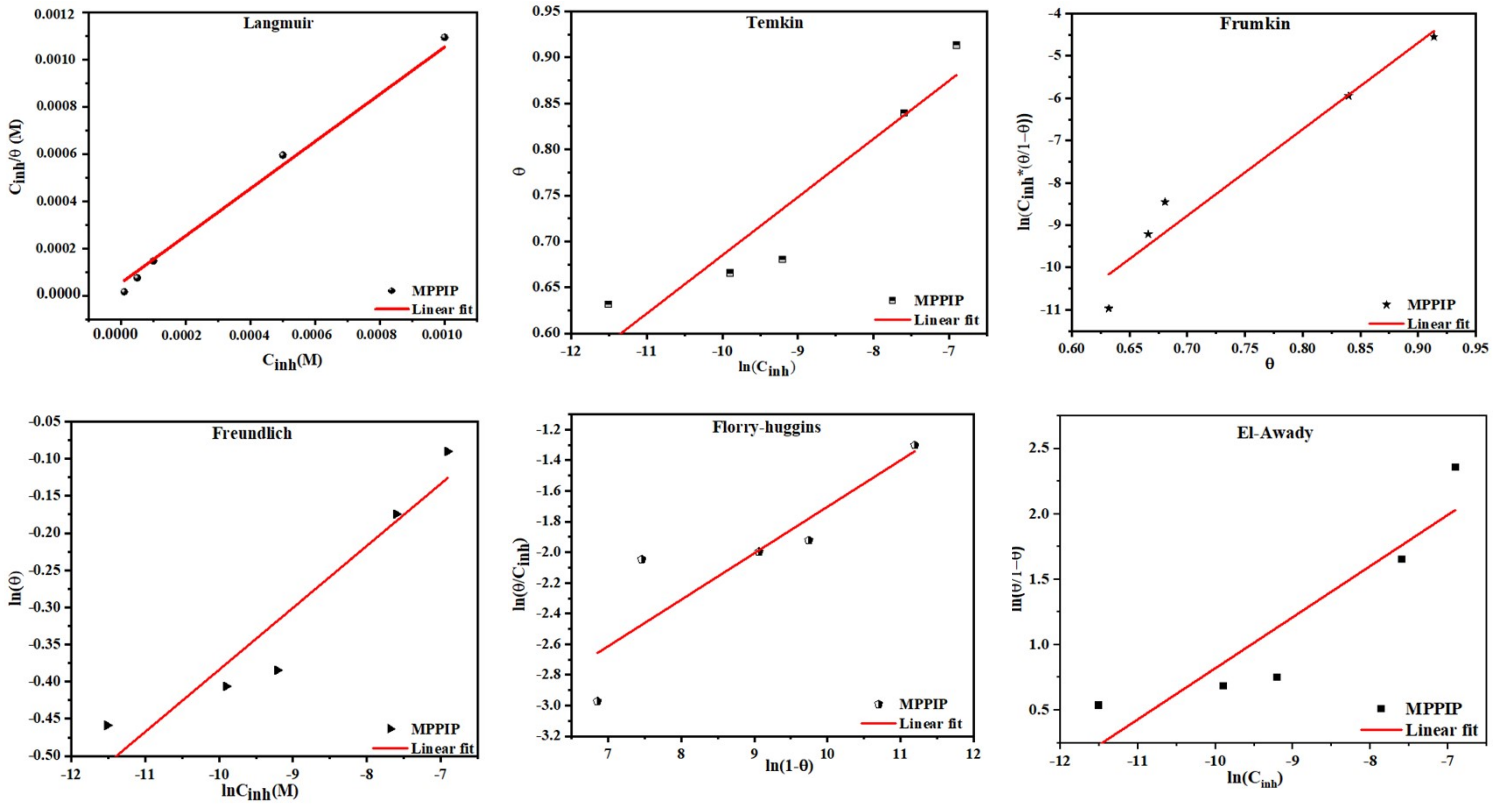

Figure S1. Representation of different adsorption isotherms for mild steel in 1M HCl with MPPIP: Temkin, Frumkin, Flory-Huggins, Freundlich, El-Awady and Langmuir models.

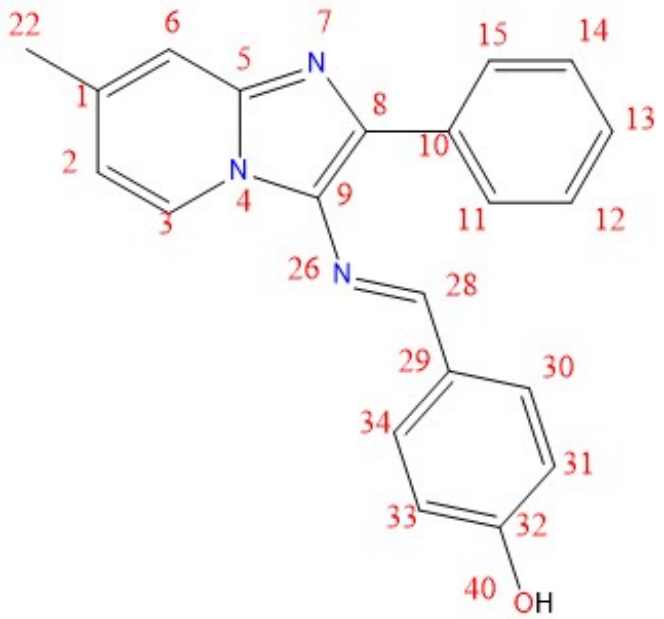

Figure S2. Molecular structure of MPPIP inhibitor with adopted atom numbering.

Table S1. The calculated values of Fukui functions, dual Fukui functions, local softness, dual local softness, electro philicity, and dual local philicity of inhibitor.

N°	Atom	MPPIP									MPPIP-H								
		f_k^-	f_k^+	Δf_k	δk+	δk-	Δδ	ω_k^+	ωk-	Δω	f_k^-	f_k^+	Δf_k	δk+	δk-	Δδ	ω_k^+	ωk-	Δω
1	C	0.040	0.017	-0.023	0.011	0.025	-0.014	0.190	*0.446*	-0.257	0.034	0.007	-0.027	0.004	0.018	-0.015	0.111	0.538	-0.427
2		0.019	0.022	0.003	0.014	0.012	0.002	0.245	*0.212*	0.033	0.017	0.008	-0.009	0.004	0.009	-0.005	0.127	0.269	-0.142
3		0.042	0.008	-0.034	0.005	0.026	-0.021	0.089	*0.469*	-0.379	0.036	0.007	-0.029	0.004	0.020	-0.016	0.111	0.569	-0.459
4	N	-0.006	0.010	0.016	0.006	-0.004	0.010	0.112	*-0.067*	0.178	-0.004	0.000	0.004	0.000	-0.002	0.002	0.000	-0.063	0.063
5	C	0.043	0.029	-0.014	0.018	0.027	-0.009	0.324	*0.480*	-0.156	0.025	0.010	-0.015	0.005	0.014	-0.008	0.158	0.395	-0.237
6		0.030	0.012	-0.018	0.007	0.019	-0.011	0.134	*0.335*	-0.201	0.038	0.008	-0.030	0.004	0.021	-0.016	0.127	0.601	-0.474
7	N	0.056	0.021	-0.035	0.013	0.035	-0.022	0.234	*0.625*	-0.390	0.026	0.008	-0.018	0.004	0.014	-0.010	0.127	0.411	-0.285
8		0.048	0.054	0.006	0.034	0.030	0.004	0.602	*0.535*	0.067	0.045	0.036	-0.009	0.020	0.024	-0.005	0.569	0.712	-0.142
9	C	0.096	0.019	-0.077	0.012	0.060	-0.048	0.212	*1.071*	-0.859	0.097	-0.003	-0.100	-0.002	0.053	-0.054	-0.047	1.534	-1.582
10		0.004	0.004	0.000	0.002	0.002	0.000	0.045	*0.045*	0.000	0.022	-0.008	-0.030	-0.004	0.012	-0.016	-0.127	0.348	-0.474
11		0.017	0.016	-0.001	0.010	0.011	-0.001	0.178	*0.190*	-0.011	0.018	-0.021	-0.039	-0.011	0.010	-0.021	-0.332	0.285	-0.617
12		0.007	0.007	0.000	0.004	0.004	0.000	0.078	*0.078*	0.000	0.018	0.008	-0.010	0.004	0.010	-0.005	0.127	0.285	-0.158
13		0.023	0.026	0.003	0.016	0.014	0.002	0.290	*0.257*	0.033	0.049	0.009	-0.040	0.005	0.027	-0.022	0.142	0.775	-0.633
14		0.007	0.006	-0.001	0.004	0.004	-0.001	0.067	*0.078*	-0.011	0.019	0.007	-0.012	0.004	0.010	-0.007	0.111	0.300	-0.190
15		0.019	0.019	0.000	0.012	0.012	0.000	0.212	*0.212*	0.000	0.031	0.010	-0.021	0.005	0.017	-0.011	0.158	0.490	-0.332
22		-0.002	-0.002	0.000	-0.001	-0.001	0.000	-0.022	*-0.022*	0.000	-0.001	-0.001	0.000	-0.001	-0.001	0.000	-0.016	-0.016	0.000
26	N	0.028	0.064	0.036	0.040	0.017	0.022	0.714	*0.312*	0.402	0.016	0.056	0.040	0.030	0.009	0.022	0.886	0.253	0.633
28	C	0.052	0.127	0.075	0.079	0.032	0.047	1.417	*0.580*	0.837	-0.004	0.173	0.177	0.094	-0.002	0.096	2.736	-0.063	2.799
29		0.011	0.000	-0.011	0.000	0.007	-0.007	0.000	*0.123*	-0.123	0.025	-0.015	-0.040	-0.008	0.014	-0.022	-0.237	0.395	-0.633
30		0.023	0.058	0.035	0.036	0.014	0.022	0.647	*0.257*	0.390	0.012	0.084	0.072	0.046	0.007	0.039	1.328	0.190	1.139
31		0.016	0.013	-0.003	0.008	0.010	-0.002	0.145	*0.178*	-0.033	0.018	0.025	0.007	0.014	0.010	0.004	0.395	0.285	0.111
32		0.030	0.057	0.027	0.036	0.019	0.017	0.636	*0.335*	0.301	0.023	0.081	0.058	0.044	0.013	0.032	1.281	0.364	0.917
33		0.018	0.018	0.000	0.011	0.011	0.000	0.201	*0.201*	0.000	0.022	0.026	0.004	0.014	0.012	0.002	0.411	0.348	0.063
34		0.026	0.043	0.017	0.027	0.016	0.011	0.480	*0.290*	0.190	0.011	0.065	0.054	0.035	0.006	0.029	1.028	0.174	0.854
40	O	0.031	0.030	-0.001	0.019	0.019	-0.001	0.335	*0.346*	-0.011	0.033	0.057	0.024	0.031	0.018	0.013	0.901	0.522	0.380