Corrosion inhibition performance of benzimidazole derivatives for protection of carbon steel in hydrochloric acid solution

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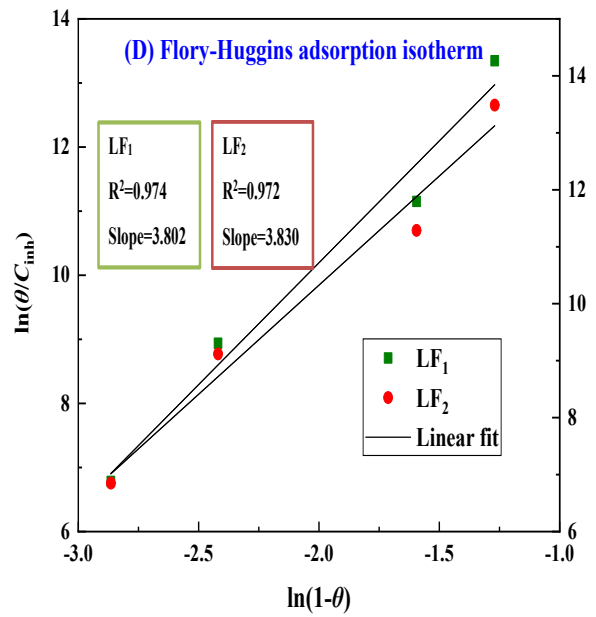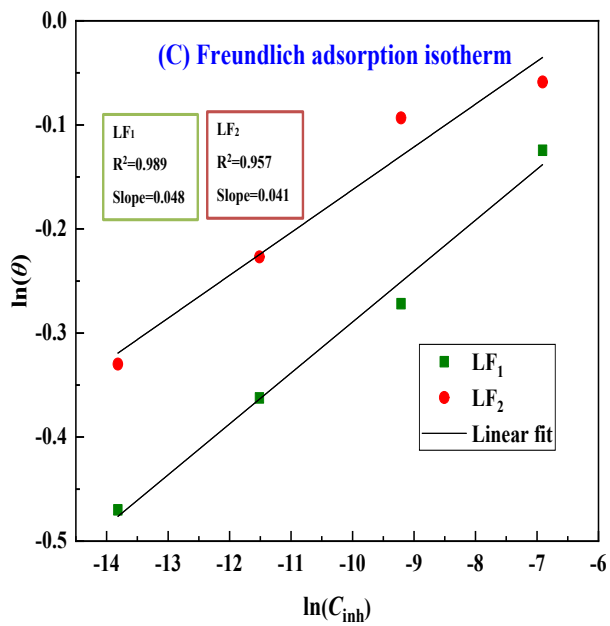[14] Chem. Depart., Faculty of Science ,Benha University, Benha, Egypt

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(A) Langmuir adsorption isotherm

LF₁
R²=0.999
Slope=1.126

LF₂
R²=0.999
Slope=0.058

(B) Temkin adsorption isotherm

LF₁
R²=0.977
Slope=1.119

LF₂
R²=0.961
Slope=0.034

(C) Freundlich adsorption isotherm

LF₁
R²=0.989
Slope=0.048

LF₂
R²=0.957
Slope=0.041

(D) Flory-Huggins adsorption isotherm

LF₁
R²=0.974
Slope=3.802

LF₂
R²=0.972
Slope=3.830
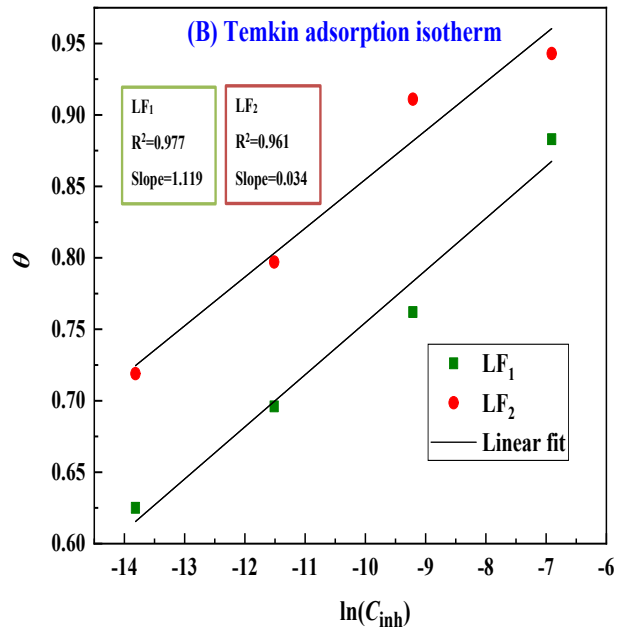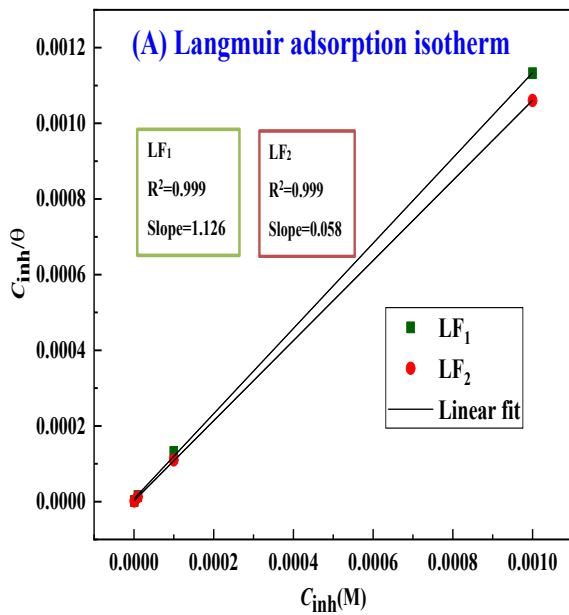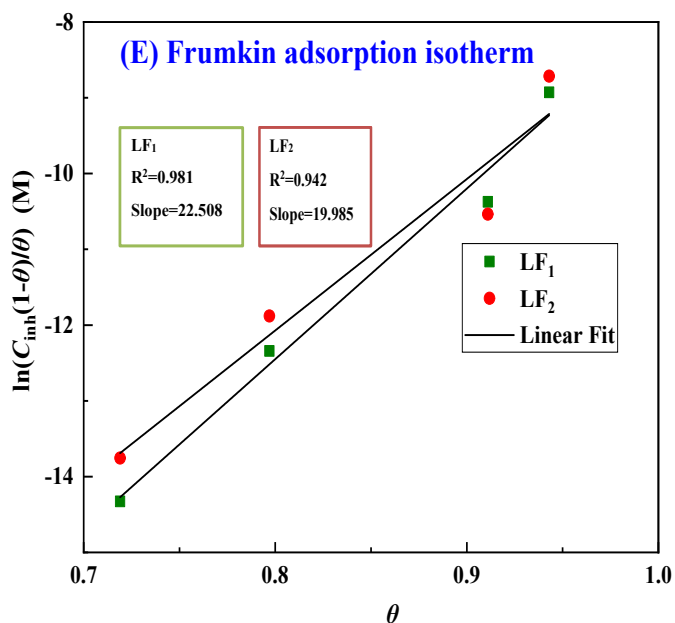
Figure S1 Plots of various adsorption isotherms for LF1 and LF2 adsorption on C.S. substrates.
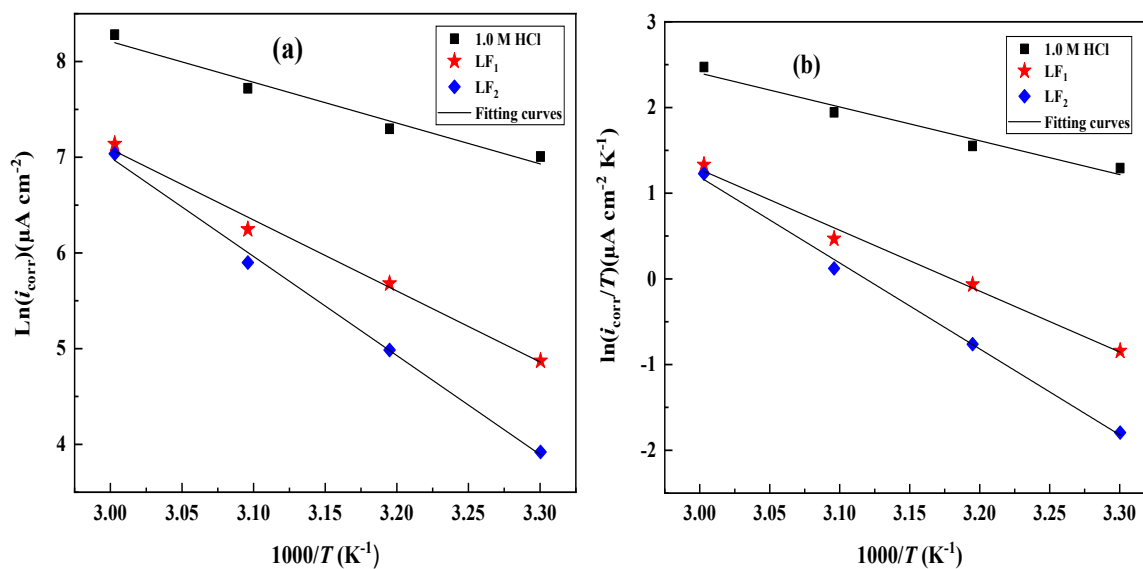
Figure S2 Variation of ln i_{corr} as a function of $1/T$ (a) and ln i_{corr}/T as a function of $1/T$ (b) of C.S. in 1.0 M HCl before and after the addition of LF$_1$ & LF$_2$ at $1*10^{-3}$ M.

Figure S3 3D-isosurface of the Fukui functions of the f_k^+, f_k^-, & Δf_k of the investigated molecules LF$_1$, & LF$_2$.

Table S1 Fukui functions of LF1 (neutral and protonated).

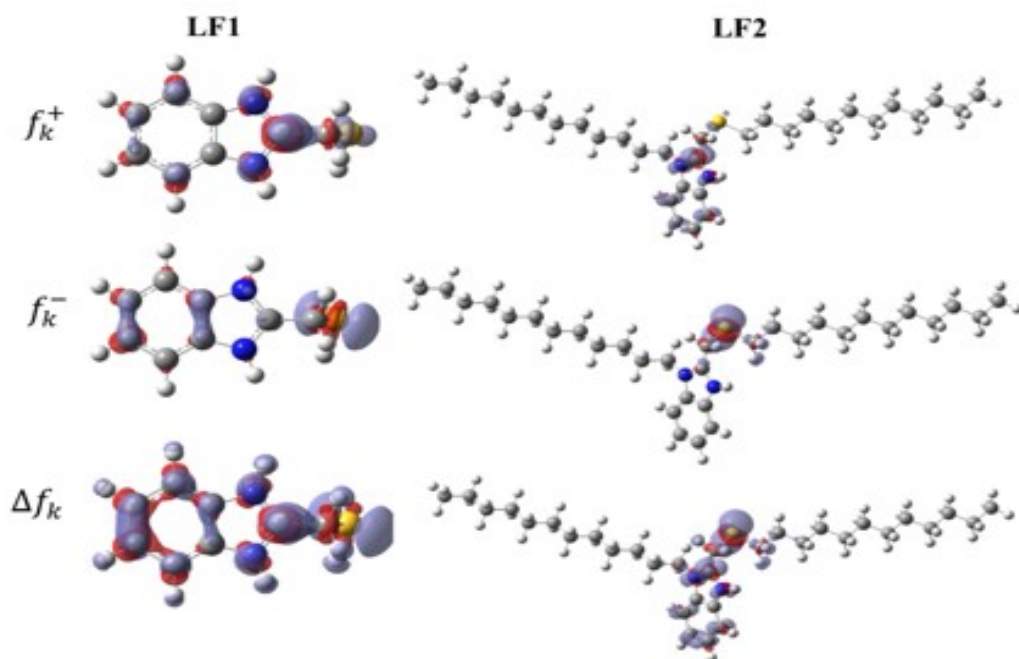| Atom	q(N)	q(N+1)	q(N-1)	f_k^-	f_k^+	Δf_k
Neutral						
C1	0.0013	-0.0343	0.0899	0.0886	0.0356	-0.0531
C2	0.0263	0	0.0851	0.0588	0.0263	-0.0325
C3	-0.0544	-0.1396	0.0215	0.0759	0.0853	0.0093
C4	-0.0514	-0.1234	0.0792	0.1306	0.072	-0.0586
C5	-0.0571	-0.108	-0.0006	0.0565	0.051	-0.0055
C6	-0.0542	-0.1439	0.0327	0.0868	0.0898	0.003
C7	0.0941	0.0116	0.1766	0.0825	0.0825	0
N12	-0.2435	-0.3092	-0.1525	0.091	0.0657	-0.0253
N13	-0.0445	-0.0791	-0.0097	0.0348	0.0346	-0.0002
C15	-0.0409	-0.0726	-0.0265	0.0144	0.0317	0.0173
S18	-0.0928	-0.2329	-0.0448	0.048	0.1401	0.0921
Protonated						
C1	0.0504	0.0252	0.1125	0.0621	0.0251	-0.037
C2	0.0499	0.0247	0.1018	0.0519	0.0252	-0.0267
C3	-0.0263	-0.0946	0.0077	0.034	0.0683	0.0343
C4	-0.0244	-0.0797	0.0556	0.08	0.0553	-0.0247
C5	-0.0242	-0.0804	0.0351	0.0593	0.0562	-0.0031
C6	-0.0265	-0.0944	0.0073	0.0338	0.0679	0.0342
C7	0.1684	0.0415	0.2059	0.0375	0.127	0.0894
N12	0.0037	-0.0597	0.0346	0.0309	0.0634	0.0326
N13	0.0063	-0.0579	0.0299	0.0235	0.0642	0.0406

					f_k^-	f_k^+	Δf_k
C15		-0.0221	-0.0562	0.0045	0.0266	0.0341	0.0075
S18		-0.0329	-0.178	0.2981	0.331	0.1451	-0.1859

Table S2 Fukui functions of LF2 (protonated).

Ato	Atom No.	q(N)	q(N+1)	q(N-1)	f_k^-	f_k^+	Δf_k
C	1	0.0424	0.0204	0.063	0.0206	0.022	0.0014
C	2	0.048	0.0219	0.0678	0.0199	0.0261	0.0062
C	3	-0.0276	-0.1035	-0.0118	0.0158	0.0759	0.0601
C	4	-0.0261	-0.0845	0.0043	0.0304	0.0583	0.0279
C	5	-0.026	-0.0873	-0.0048	0.0212	0.0612	0.04
C	6	-0.0303	-0.1025	-0.0145	0.0158	0.0722	0.0564
C	7	0.1588	0.0409	0.1654	0.0066	0.1178	0.1113
N	12	0.0286	-0.0186	0.0438	0.0152	0.0472	0.032
N	13	0.0003	-0.0581	0.0145	0.0142	0.0584	0.0443
C	15	-0.0338	-0.0601	-0.0009	0.0329	0.0263	-0.0066
S	18	-0.0192	-0.1104	0.4366	0.4558	0.0912	-0.3646
C	19	-0.0426	-0.0494	-0.0051	0.0375	0.0068	-0.0308
C	20	-0.0432	-0.0485	-0.0334	0.0098	0.0054	-0.0044
C	23	-0.0412	-0.0436	-0.0347	0.0064	0.0024	-0.004
C	26	-0.044	-0.045	-0.0406	0.0034	0.0009	-0.0024
C	31	-0.0455	-0.046	-0.0438	0.0017	0.0005	-0.0012
C	32	-0.046	-0.0462	-0.0451	0.0008	0.0003	-0.0006
C	35	-0.0464	-0.0465	-0.0459	0.0004	0.0001	-0.0003
C	38	-0.0464	-0.0464	-0.0461	0.0002	0.0001	-0.0002
C	43	-0.0465	-0.0465	-0.0464	0.0001	0	-0.0001
C	44	-0.0467	-0.0467	-0.0466	0.0001	0	0
C	47	-0.0448	-0.0448	-0.0447	0	0	0
C	50	-0.0861	-0.0861	-0.086	0	0	0
C	56	0.0246	0.0141	0.0309	0.0064	0.0104	0.0041
C	57	-0.0428	-0.0484	-0.04	0.0028	0.0056	0.0028
C	60	-0.0393	-0.0428	-0.0377	0.0017	0.0035	0.0018
C	63	-0.0428	-0.0445	-0.0418	0.001	0.0017	0.0007
C	68	-0.0449	-0.0458	-0.0444	0.0005	0.0009	0.0003
C	69	-0.0458	-0.0463	-0.0455	0.0003	0.0004	0.0001
C	72	-0.0462	-0.0464	-0.046	0.0001	0.0002	0.0001
C	75	-0.0464	-0.0465	-0.0463	0.0001	0.0001	0
C	80	-0.0464	-0.0465	-0.0464	0	0.0001	0
C	81	-0.0467	-0.0467	-0.0466	0	0	0
C	84	-0.0448	-0.0448	-0.0447	0	0	0
C	87	-0.0861	-0.0861	-0.086	0	0	0