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

Supplementary Information

Newly synthesized quercetin derivatives as corrosion inhibitor for mild steel in 1 M HCl: combined experimental and theoretical investigation

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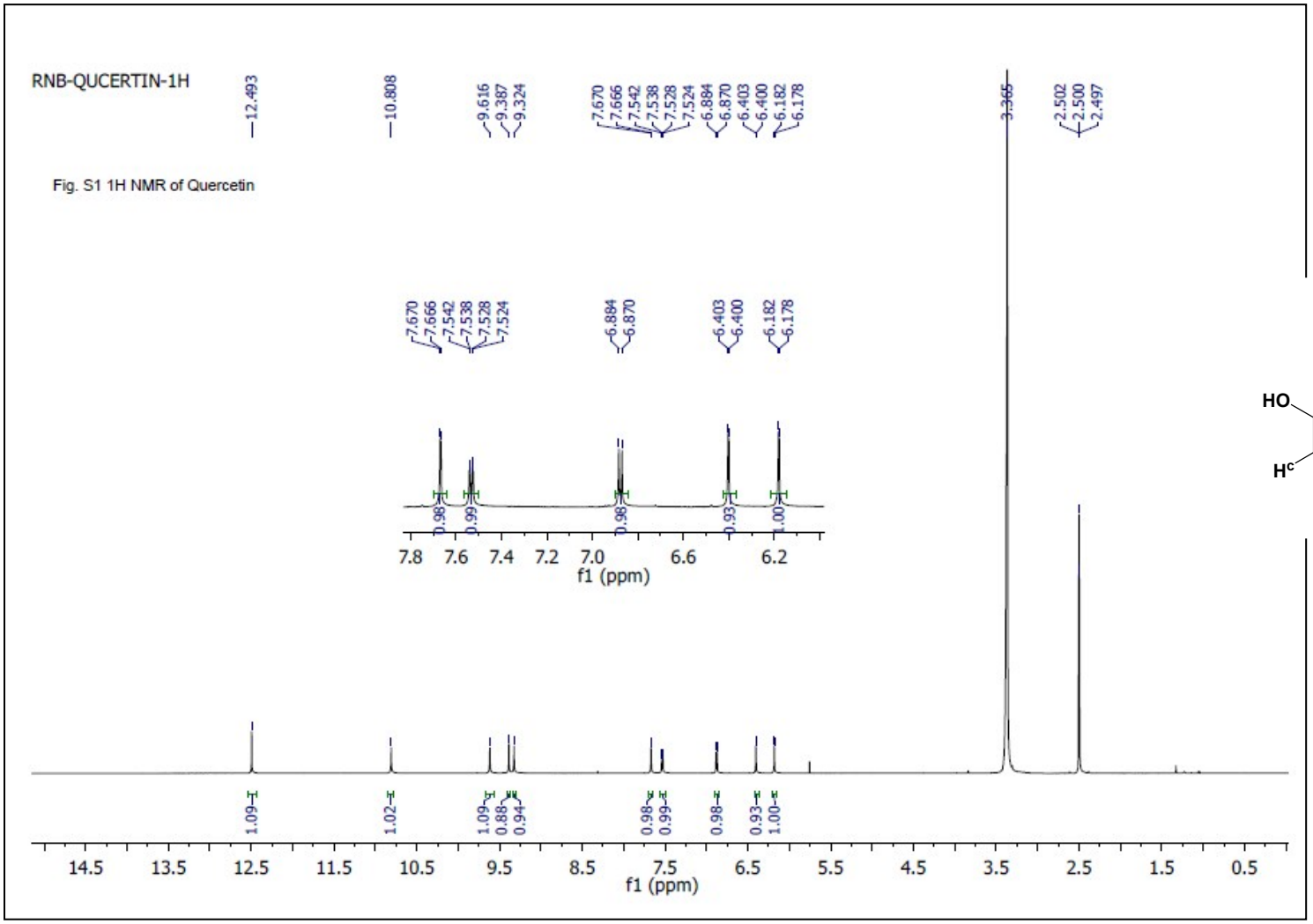
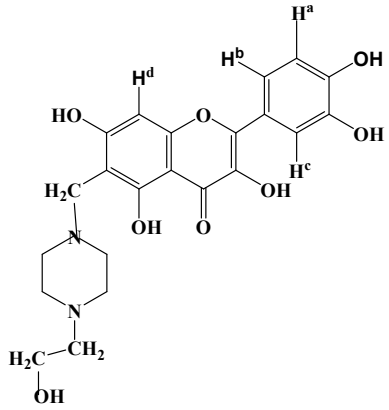


Fig. S1 ^{1}H NMR of Quercetin



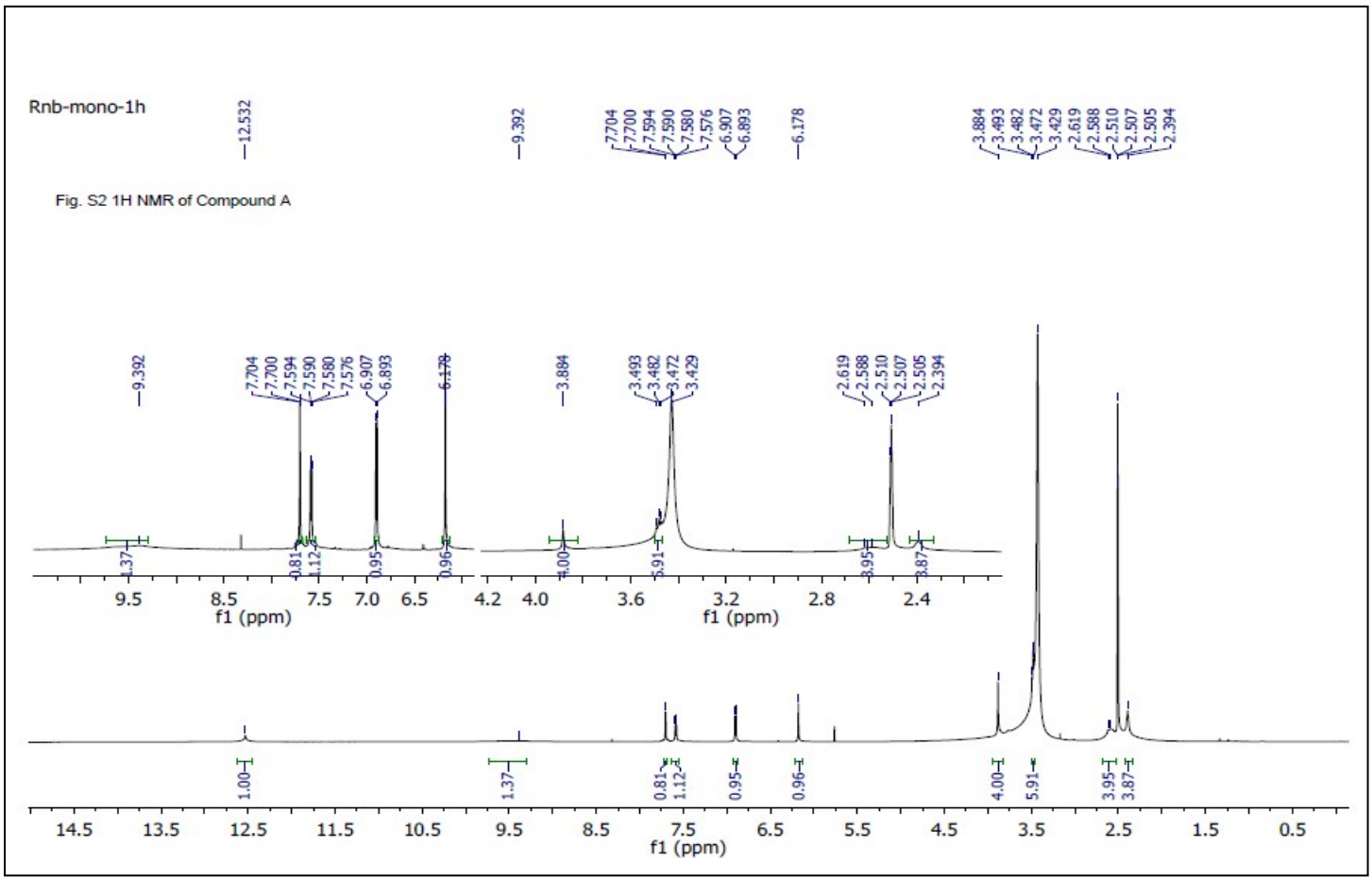
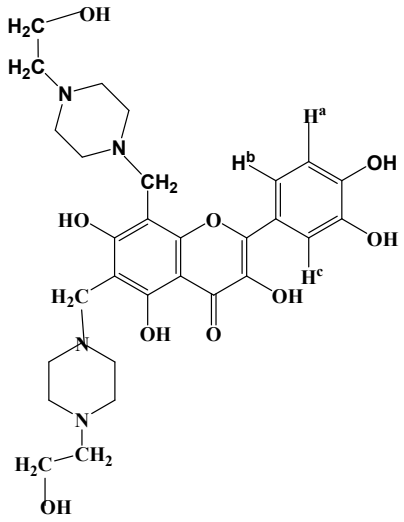


Fig. S2 ^{1}H NMR of Compound A



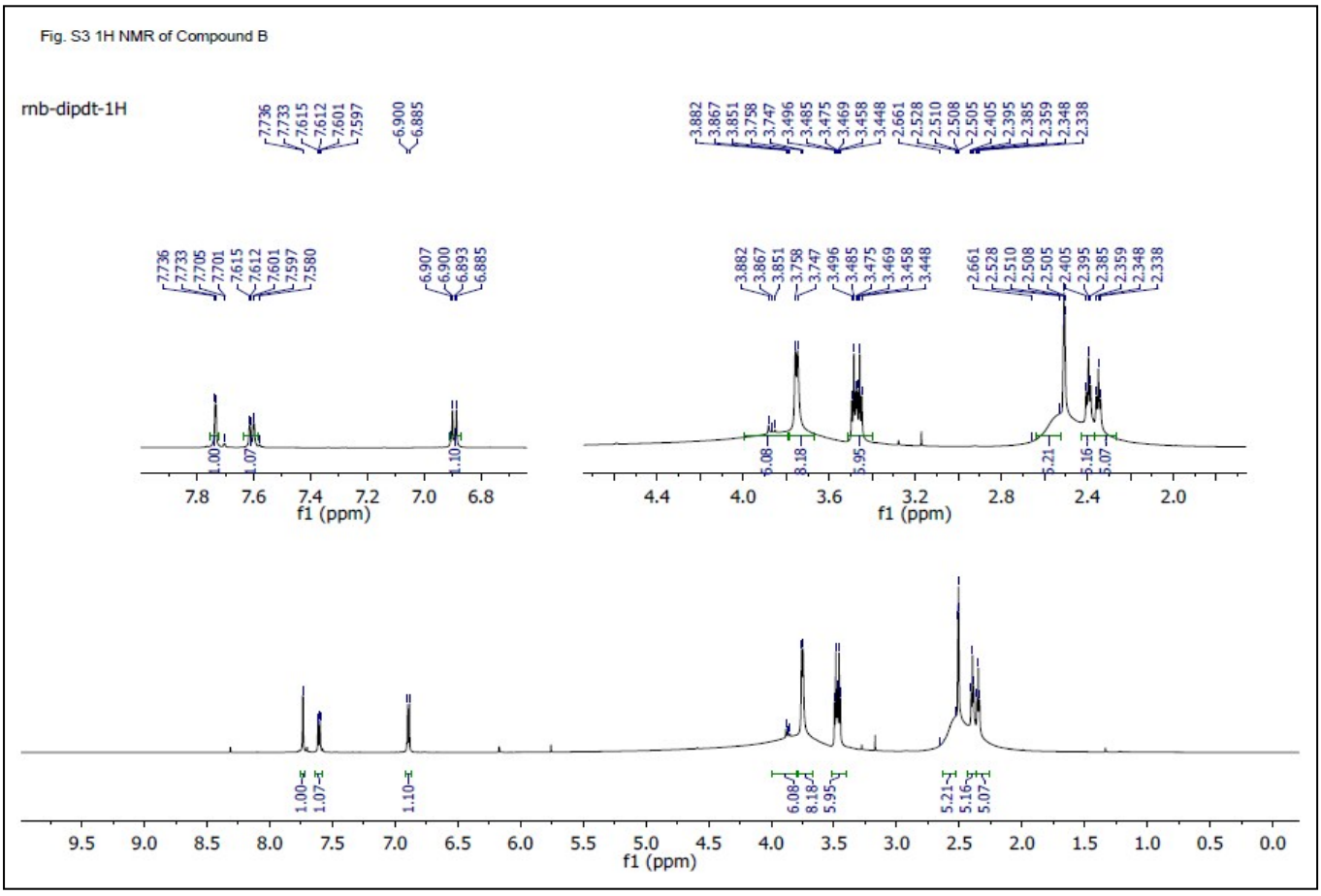


Fig. S3 ^{1}H NMR of Compound B

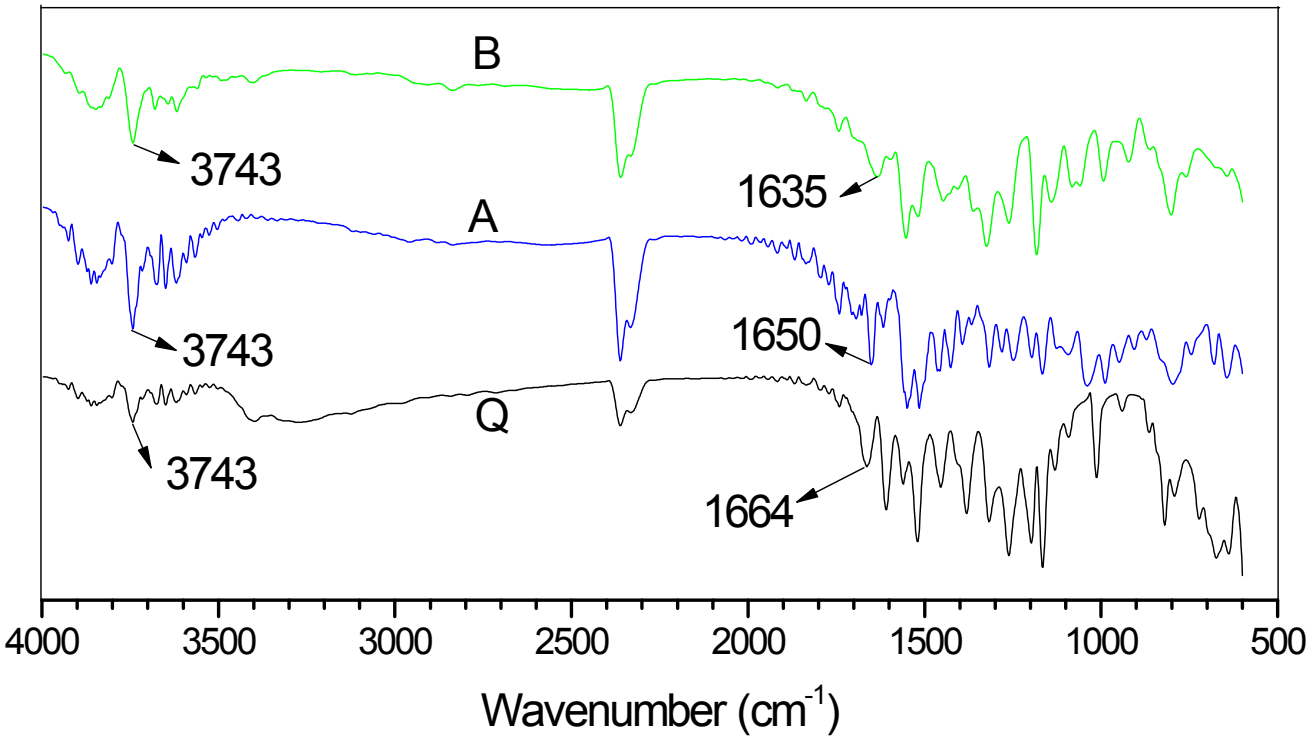


Fig. S4 FTIR spectra of Quercetin (Q), Compound A (A) and Compound B (B).

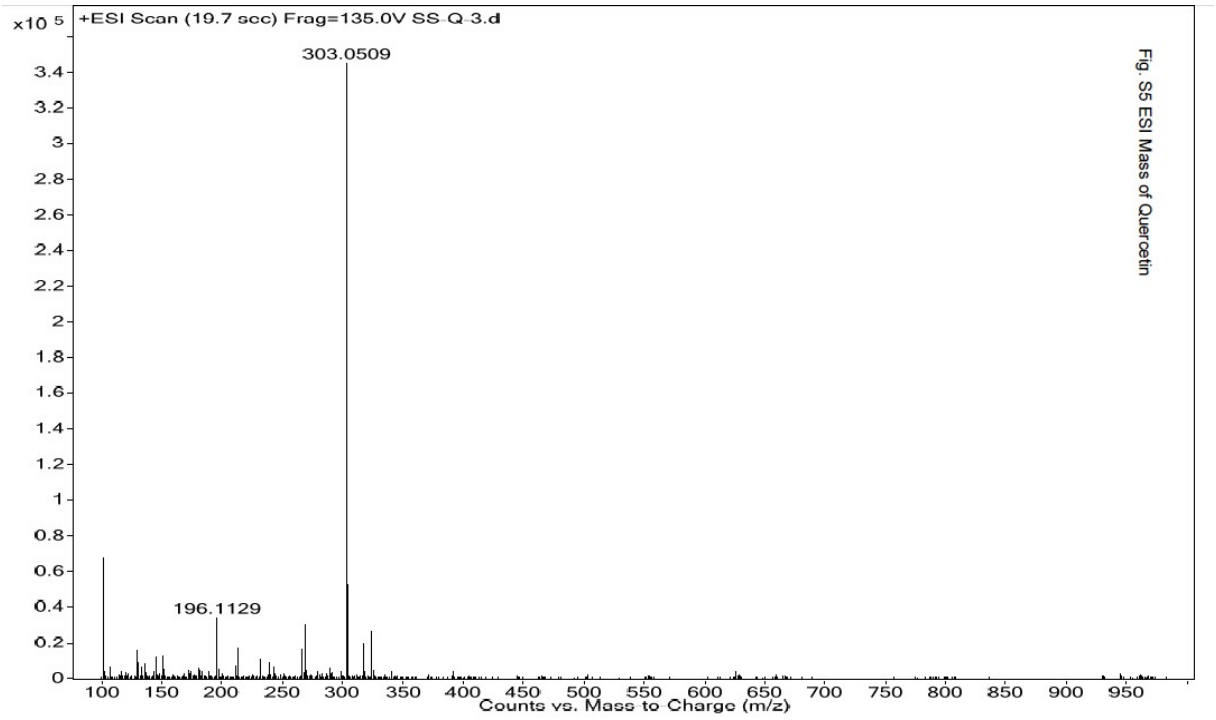


Fig. S5 ESI-Mass spectrum of Quercetin

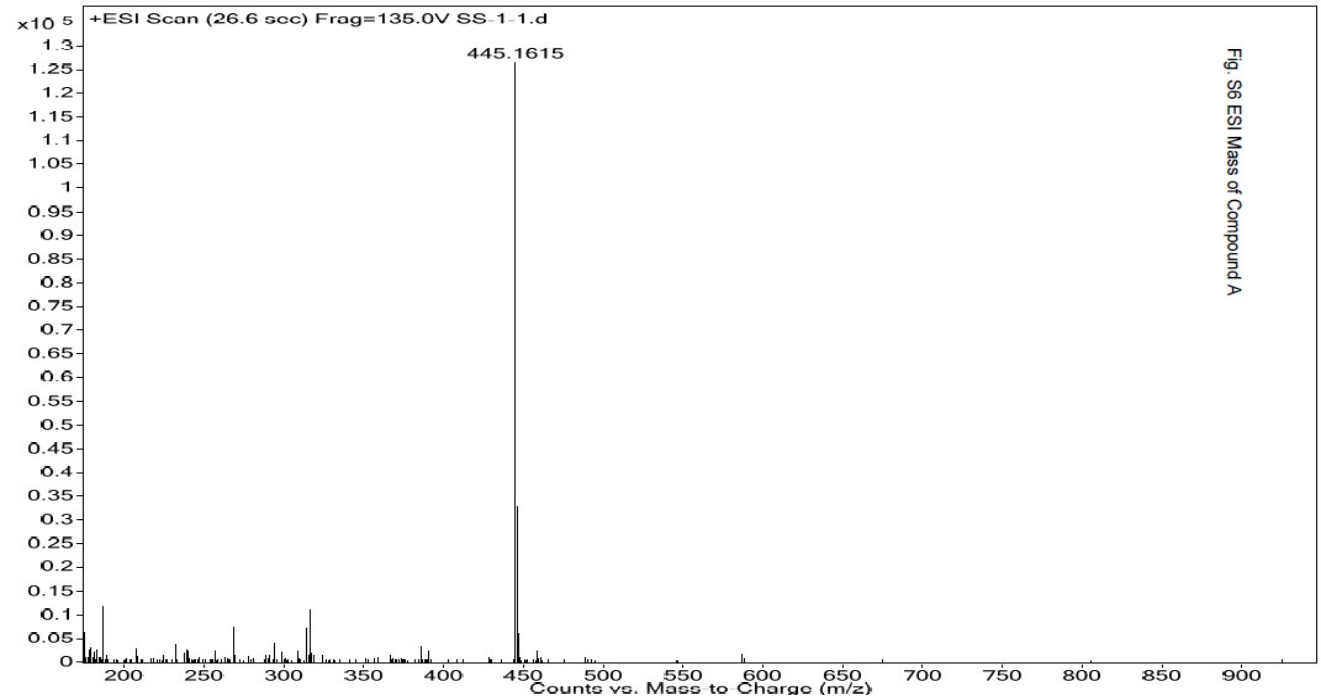


Fig. S6 ESI-Mass spectrum of Compound A

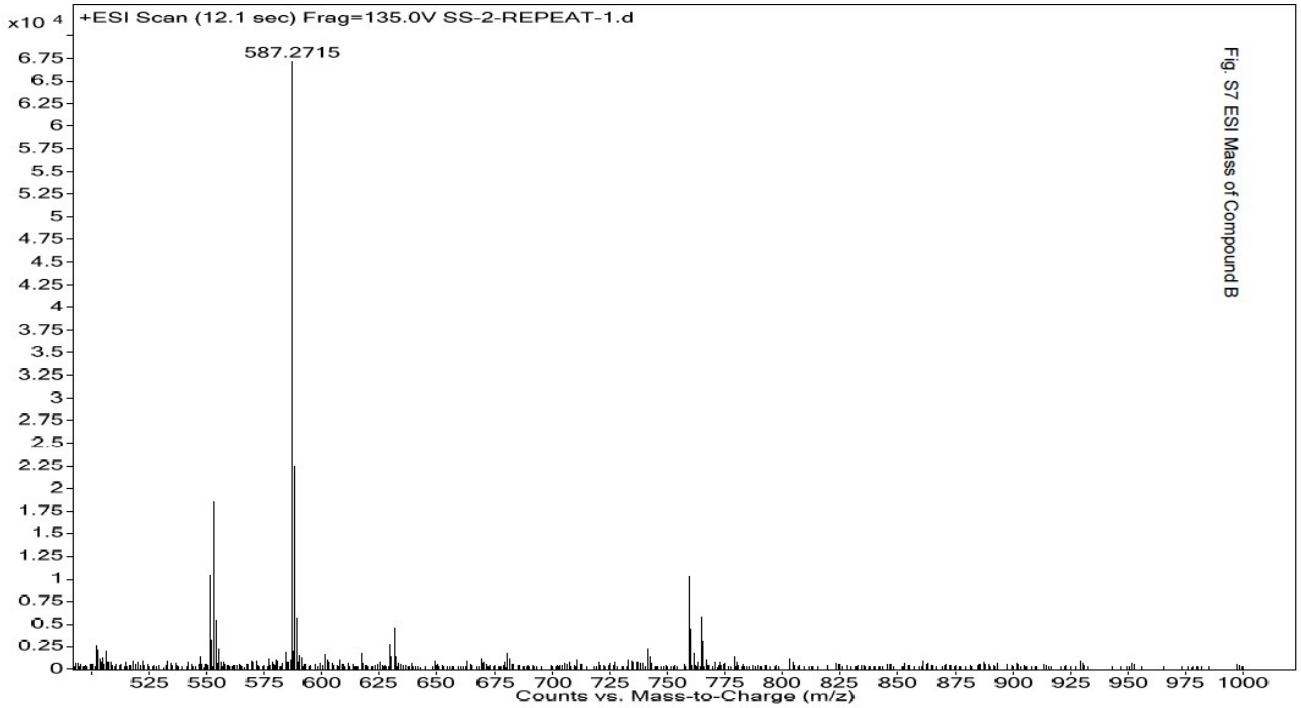


Fig. S7 ESI-Mass spectrum of Compound B

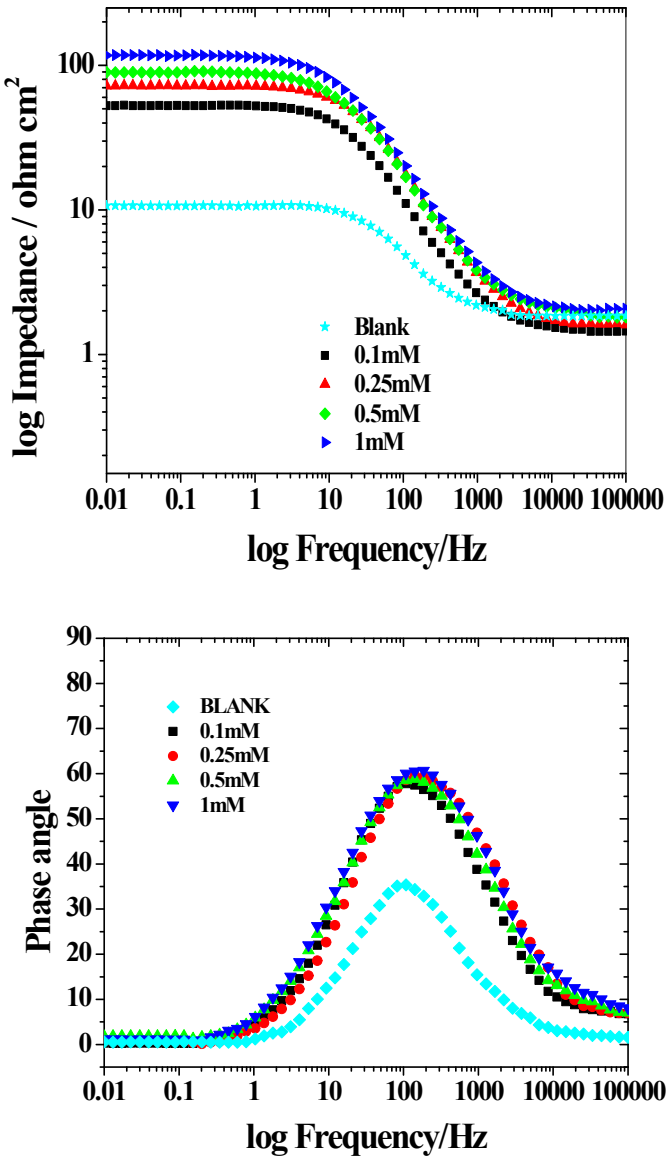
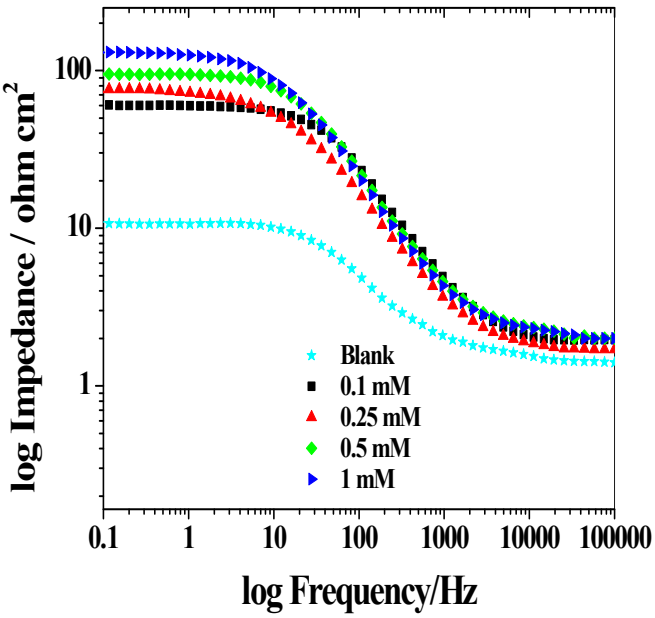


Fig. S8 Bode impedance plot (up)and phase angle plot (down) in absence and presence of compound A



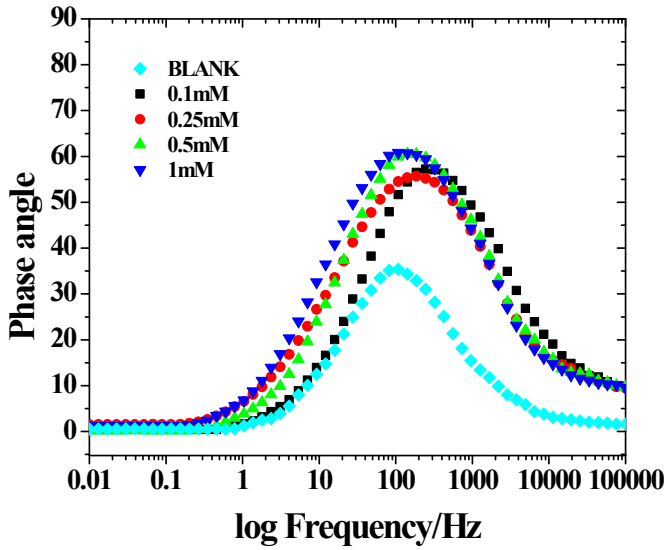


Fig. S9 Bode impedance plot (up)and phase angle plot (down) in absence and presence of compound B

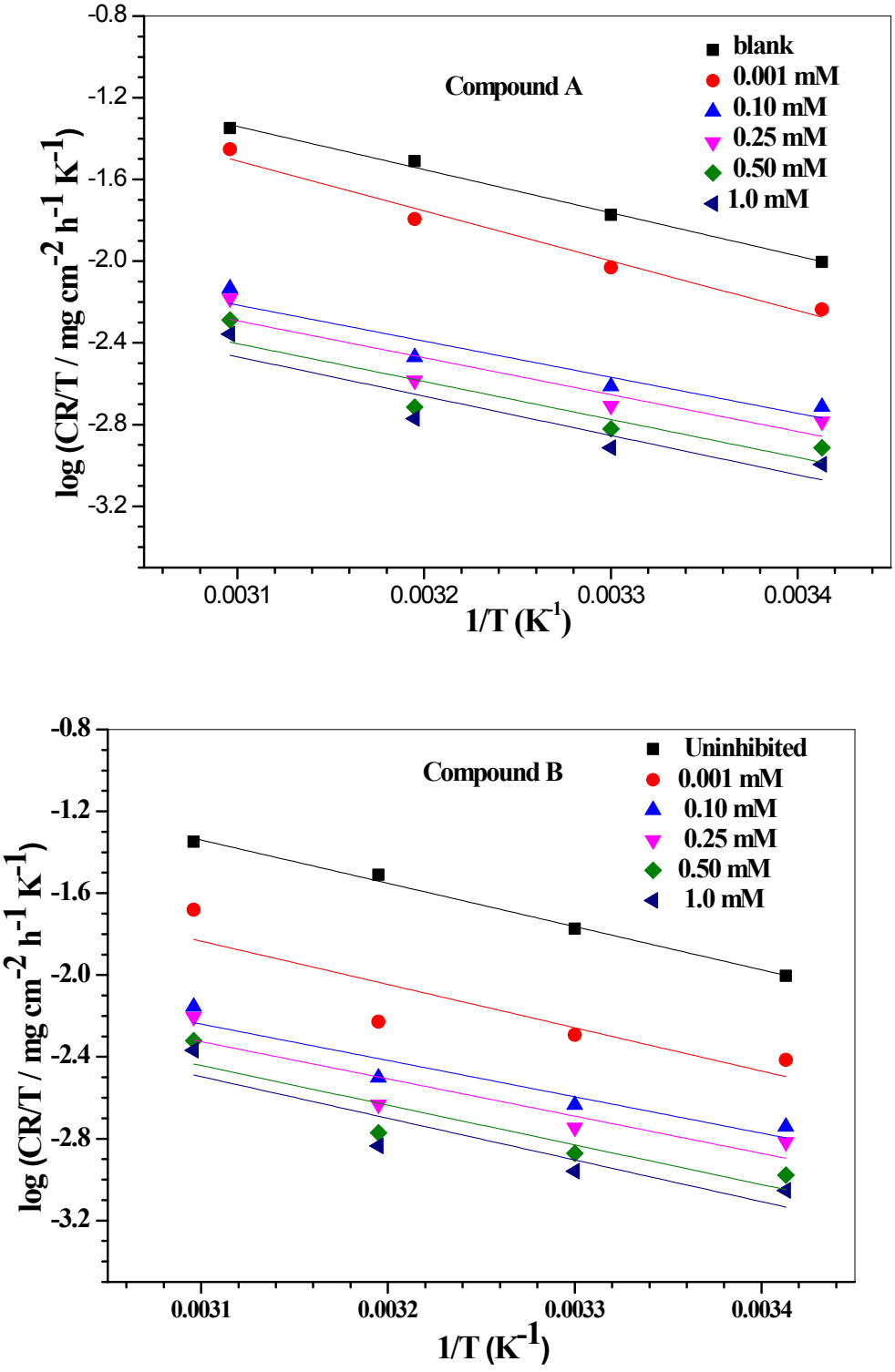
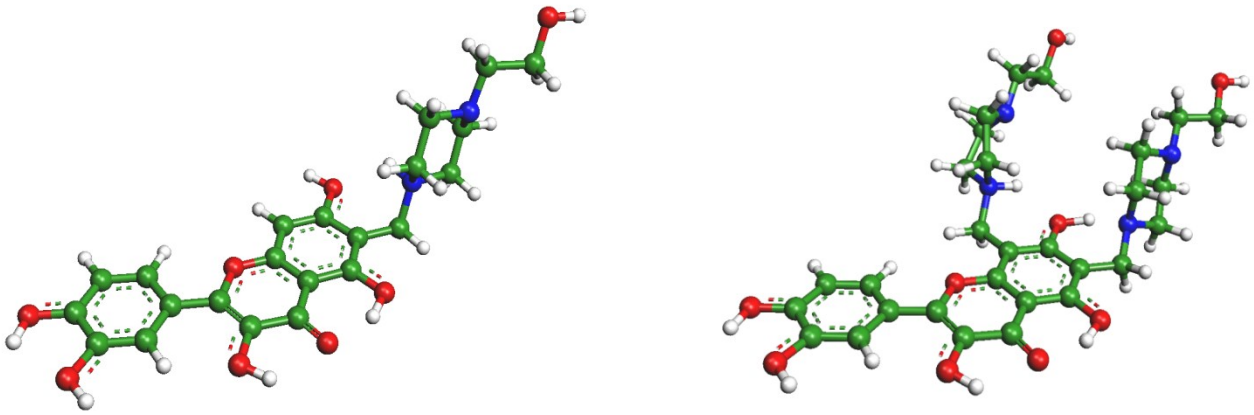
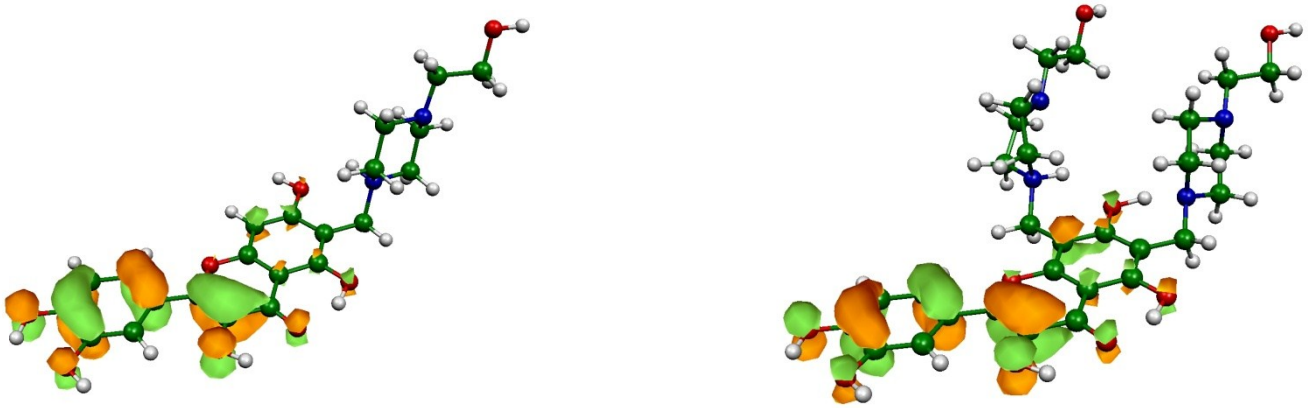


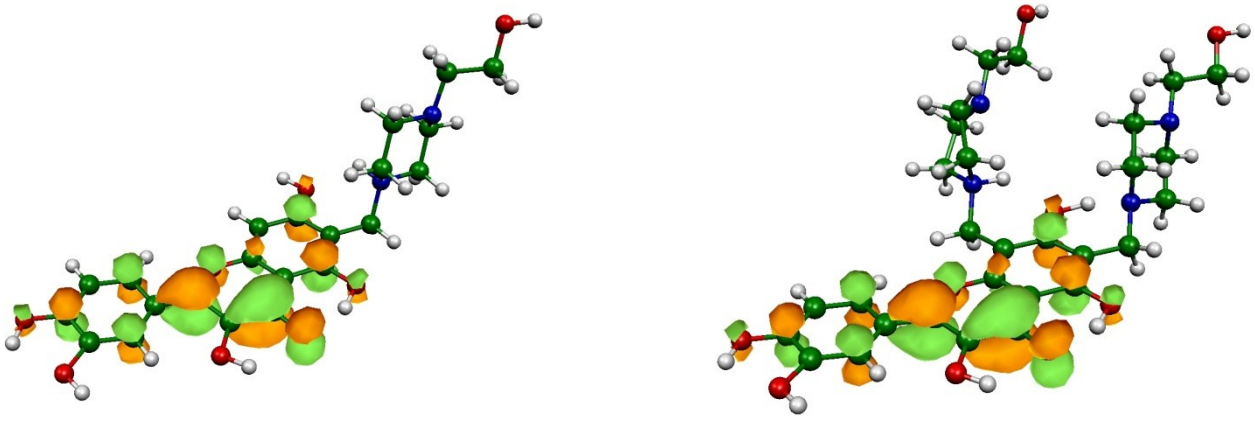
Fig. S10 Arrhenius plots for mild steel in 1 M HCl solution in absence and presence of compound A (up) and compound B (down) (following eqn. 18)



OPTIMIZED GEOMETRY



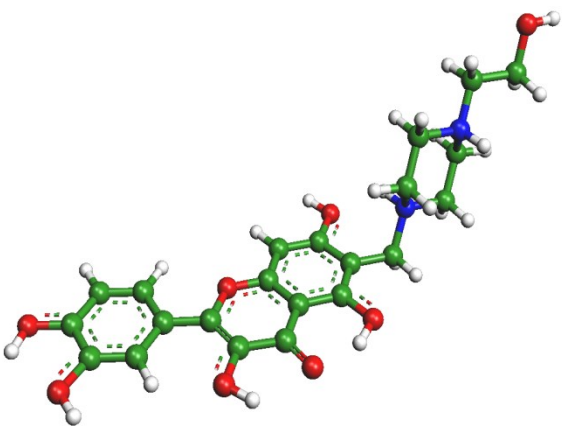
HOMO

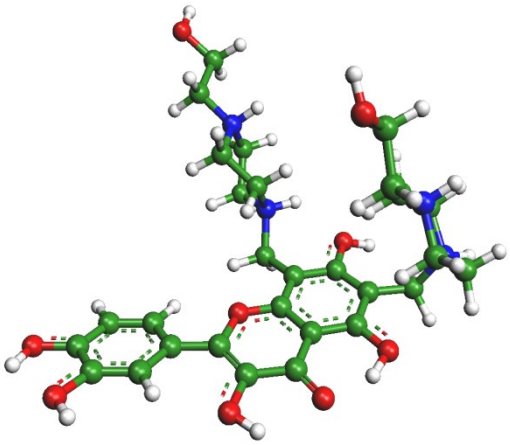


LUMO

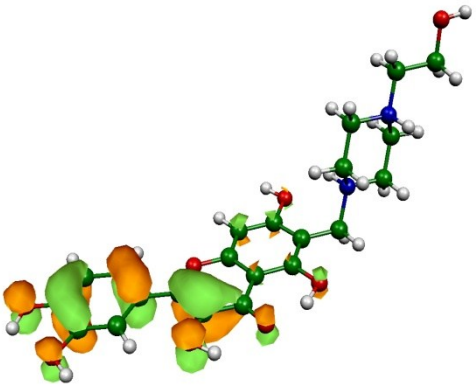
Compound A **Compound B**

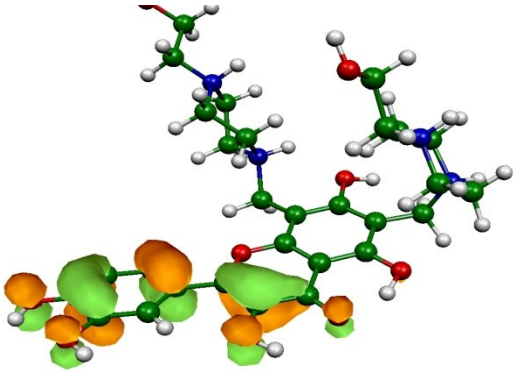
Fig. S11 Optimized geometry and electron distribution in HOMO and LUMO for compound A and B in their mono-protonated state



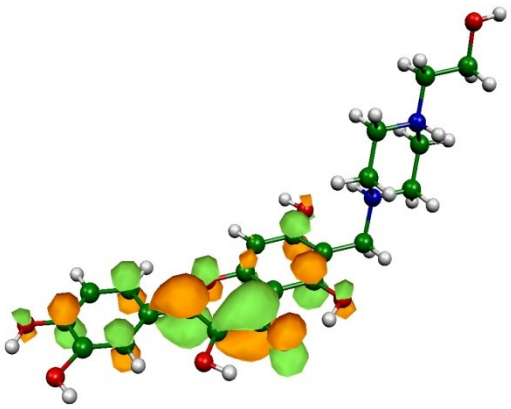


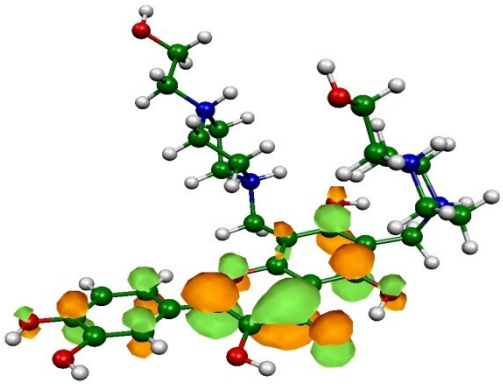
OPTIMIZED GEOMETRY





HOMO





LUMO

Compound A **Compound B**

Fig. S12 Optimized geometry and electron distribution in HOMO and LUMO for compound A and B in their fully protonated state

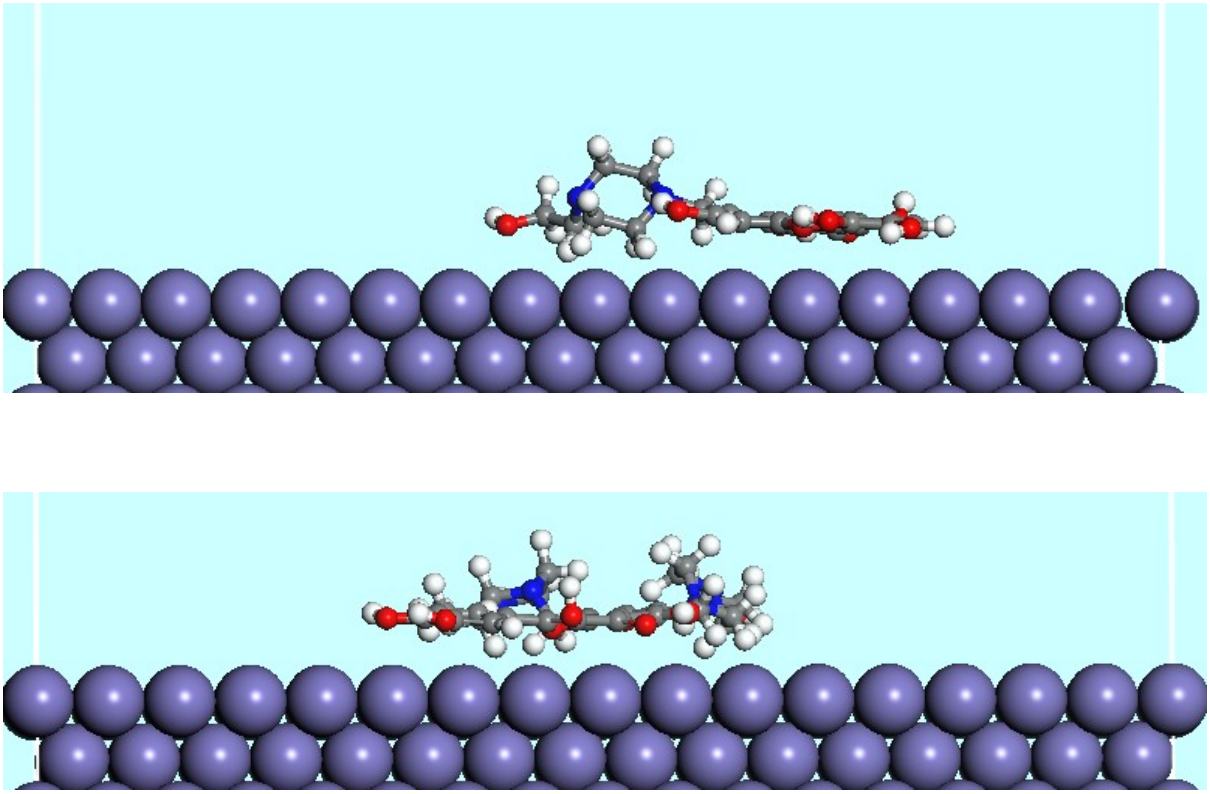
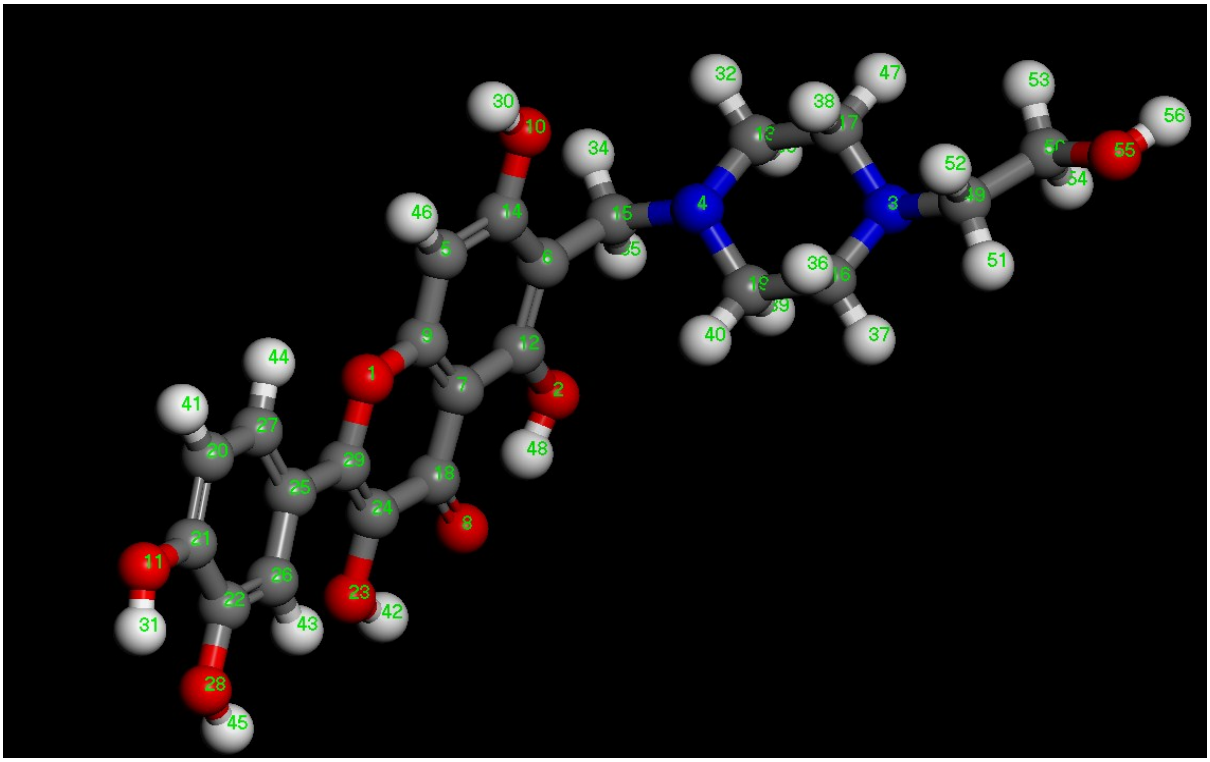


Fig. S13 Closer side view of equilibrium adsorption configurations of compound A (up) and compound B (down) on Fe (1 1 0) surface obtained by molecular dynamics simulation. Water molecules are deactivated for claririty.

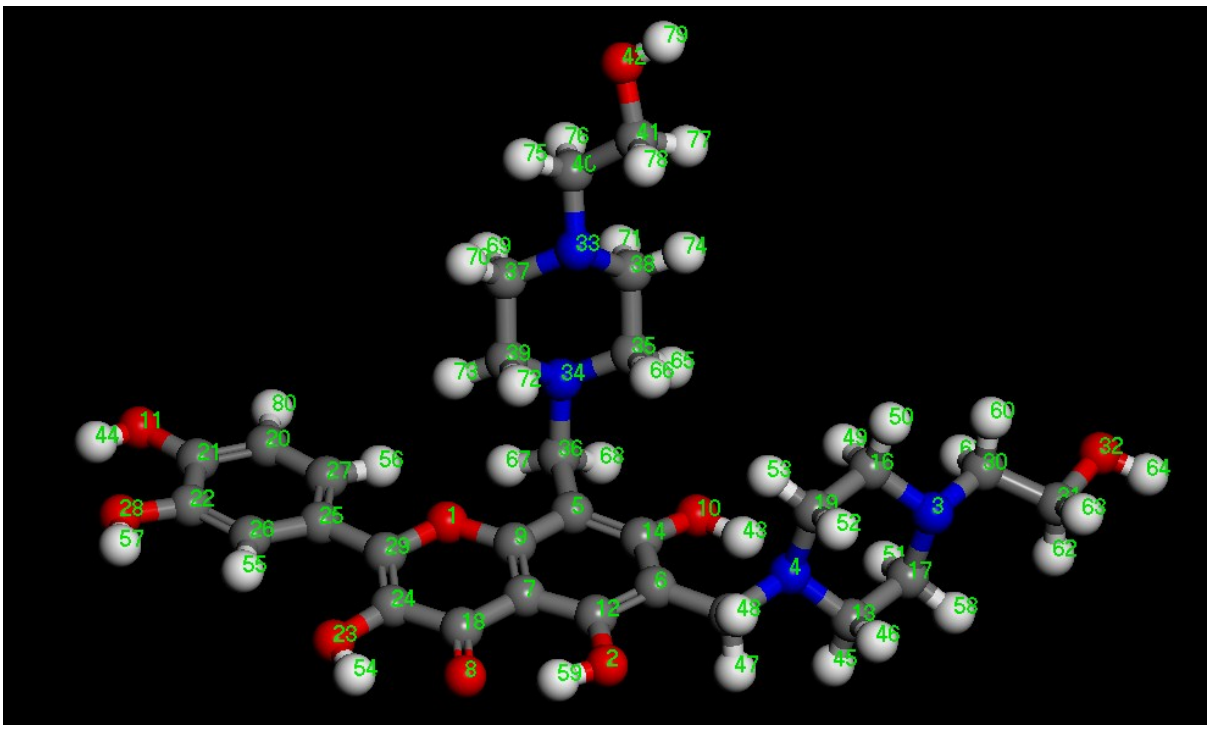
Table S1 Corrosion rate of mild steel in 1 M HCl in presence and absence of Quercetin derivatives at different exposure times at 303K

Exposure Time (h)	Inhibitor	Corrosion Rate (mg cm^{-2} h^{-1})	η_w%
6	Uninhibited	5.098	
	Compound A	0.370	92.7
	Compound B	0.333	93.5
24	Uninhibited	8.444	
	Compound A	0.518	93.8
	Compound B	0.432	94.9
48	Uninhibited	9.777	
	Compound A	0.530	94.3
	Compound B	0.456	95.3
72	Uninhibited	11.666	
	Compound A	0.6913	94.1
	Compound B	0.5802	95.0
96	Uninhibited	15.209	
	Compound A	1.444	90.5
	Compound B	1.333	91.1

Table S2. Calculated Fukui functions of the atoms present in Quercetin derivatives



Numbering of atoms of Compound A



Numbering of atoms of compound B

Compound A			Compound B		
Atom	f_k^+	f_k^-	Atom	f_k^+	f_k^-
O (1)	0.045	0.016	O (1)	0.037	0.017
O (2)	0.031	0.022	O (2)	0.032	0.032
N (3)	0	0.029	N (3)	0	0.007
N (4)	0.001	0.074	N (4)	0.001	0.001
C (5)	0.026	0.027	C (5)	0.018	0.036
C (6)	0.021	0.008	C (6)	0.023	0.015
C (7)	0.022	0.015	C (7)	0.023	0.023
O (8)	0.1	0.027	O (8)	0.098	0.028
C (9)	0.026	0.011	C (9)	0.021	0.012
O (10)	0.026	0.016	O (10)	0.026	0.026
O (11)	0.029	0.04	O (11)	0.029	0.035
C (12)	0.033	0.017	C (12)	0.035	0.026
C (13)	0.002	0.014	C (13)	0.001	0.002
C (14)	0.037	0.016	C (14)	0.033	0.022
C (15)	0.004	0.013	C (15)	0.005	0.004
C (16)	0.001	0.009	C (16)	0	0.001
C (17)	0.001	0.009	C (17)	0.001	0.002
C (18)	0.096	0.015	C (18)	0.094	0.017
C (19)	0.001	0.013	C (19)	0	0.001
C (20)	0.023	0.024	C (20)	0.023	0.022
C (21)	0.041	0.038	C (21)	0.042	0.035
C (22)	0.019	0.025	C (22)	0.019	0.021
O (23)	0.028	0.046	O (23)	0.029	0.051
C (24)	0.04	0.049	C (24)	0.042	0.054
C (25)	0.023	0.03	C (25)	0.023	0.024
C (26)	0.036	0.017	C (26)	0.037	0.016
C (27)	0.04	0.032	C (27)	0.038	0.027
O (28)	0.013	0.022	O (28)	0.014	0.018
C (29)	0.084	0.028	C (29)	0.082	0.033
H (30)	0.012	0.008	C (30)	0	0.001
H (31)	0.01	0.013	C (31)	0	0.001
H (32)	0.002	0.013	O (32)	0	0.001
H (33)	0.002	0.027	N (33)	0	0.018
H (34)	0.007	0.012	N (34)	0.003	0.062
H (35)	0.006	0.022	C (35)	0.001	0.01
H (36)	0.001	0.014	C (36)	0.004	0.012
H (37)	0.001	0.011	C (37)	0.001	0.007
H (38)	0.001	0.014	C (38)	0.001	0.007
H (39)	0.002	0.026	C (39)	0.001	0.01
H (40)	0.001	0.012	C (40)	0	0.004
H (41)	0.014	0.013	C (41)	0	0.002

H (42)	0.017	0.016	O (42)	0	0.002
H (43)	0.016	0.01	H (43)	0.005	0.006
H (44)	0.019	0.014	H (44)	0.011	0.012
H (45)	0.007	0.009	H (45)	0.002	0.002
H (46)	0.016	0.012	H (46)	0.002	0.003
H (47)	0.001	0.01	H (47)	0.008	0.006
H (48)	0.015	0.008	H (48)	0.007	0.006
C (49)	0	0.006	H (49)	0.001	0.002
C (50)	0	0.002	H (50)	0.001	0.002
H (51)	0	0.005	H (51)	0.001	0.002
H (52)	0	0.01	H (52)	0.003	0.003
H (53)	0	0.002	H (53)	0.001	0.001
H (54)	0	0.003	H (54)	0.018	0.018
O (55)	0	0.003	H (55)	0.016	0.01
H (56)	0	0.002	H (56)	0.016	0.011
			H (57)	0.007	0.008
			H (58)	0.001	0.002
			H (59)	0.015	0.01
			H (60)	0	0.001
			H (61)	0	0.002
			H (62)	0	0
			H (63)	0	0.001
			H (64)	0	0
			H (65)	0.002	0.01
			H (66)	0.001	0.017
			H (67)	0.006	0.012
			H (68)	0.007	0.013
			H (69)	0.002	0.011
			H (70)	0.002	0.009
			H (71)	0.002	0.011
			H (72)	0.002	0.018
			H (73)	0.001	0.008
			H (74)	0.001	0.008
			H (75)	0.001	0.004
			H (76)	0.001	0.007
			H (77)	0	0.002
			H (78)	0	0.002
			H (79)	0	0.001
			H (80)	0.014	0.012