SUPPLEMENTARY INFORMATION

Adsorption and anti-corrosion characteristics of Vanillin Schiff bases on mild steel in 1M HCl: Experimental and theoretical study

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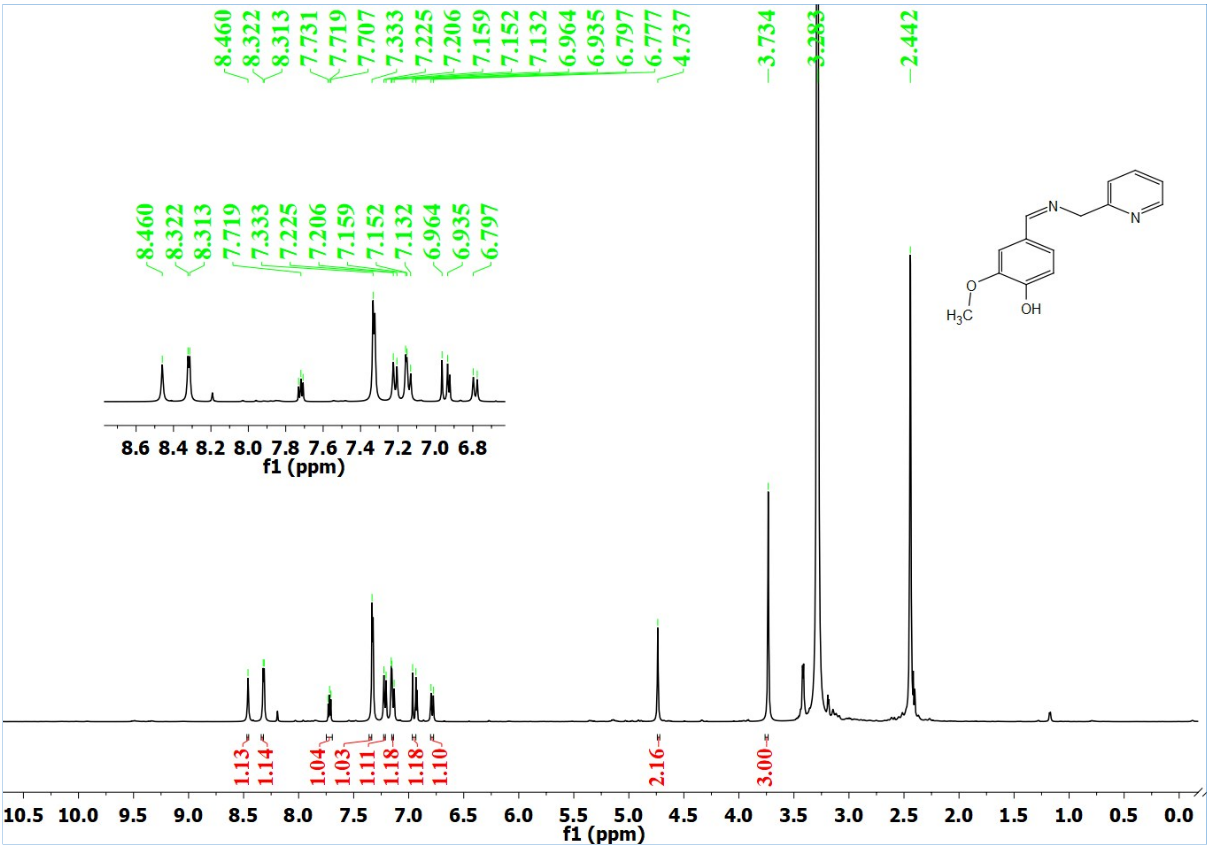


Fig. S1 [1]H NMR of Compound A

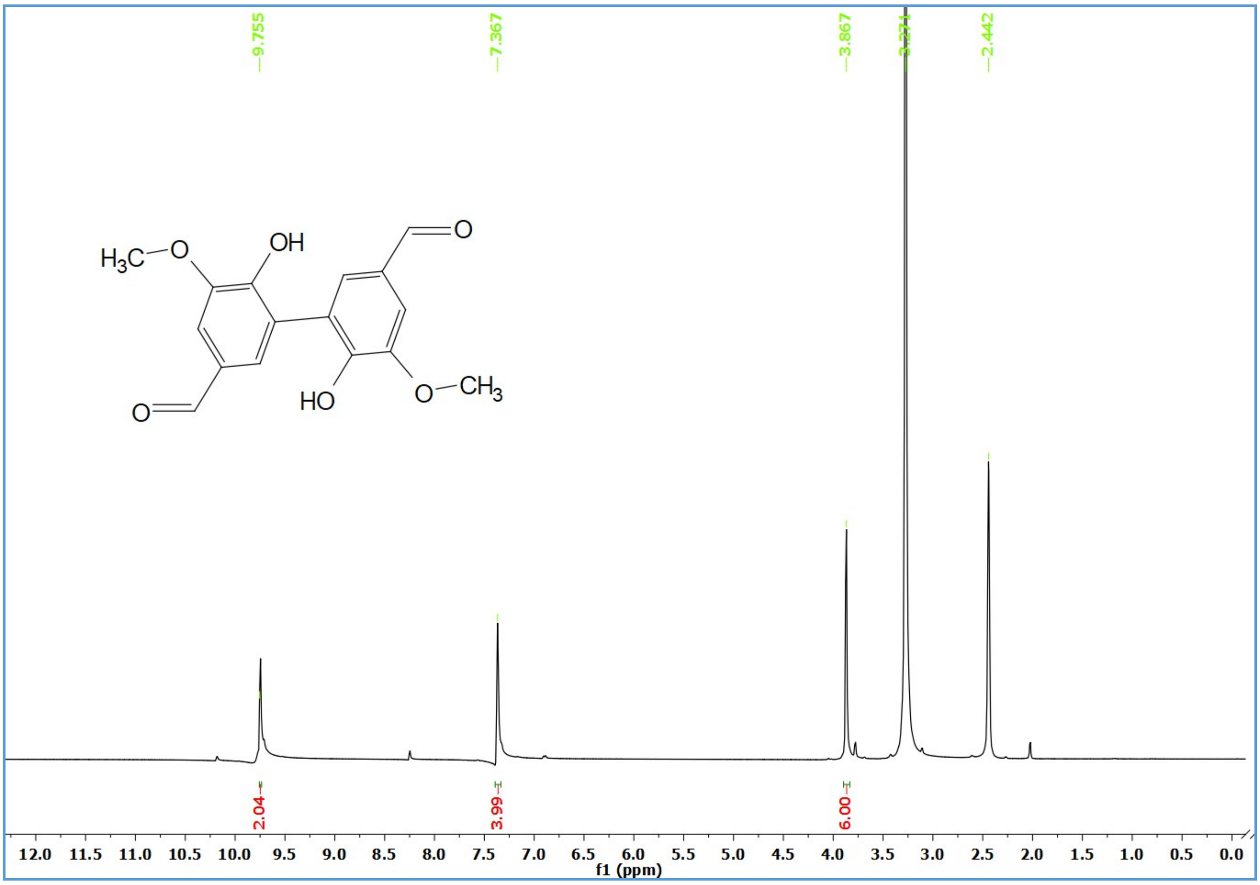


Fig. S2 ^{1}H NMR of divanillin

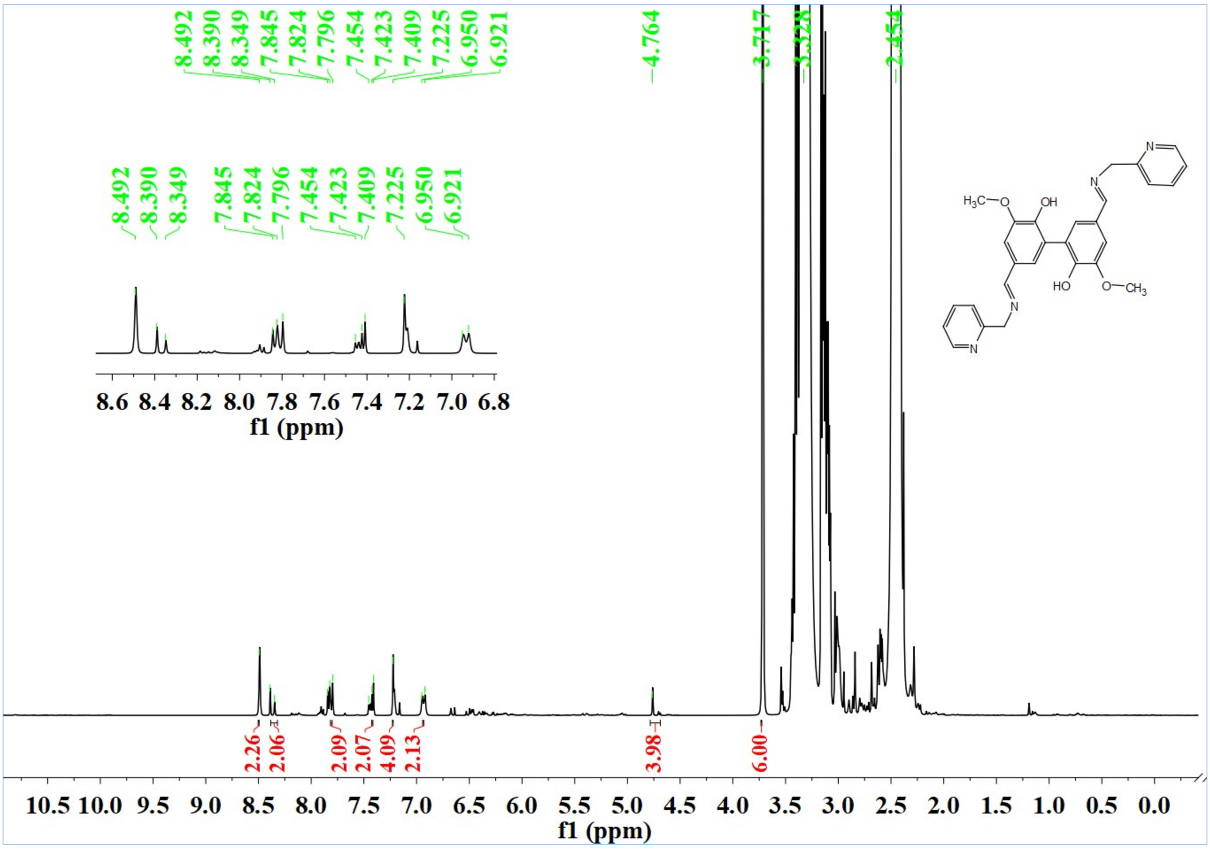


Fig. S3 ^{1}H NMR of Compound B

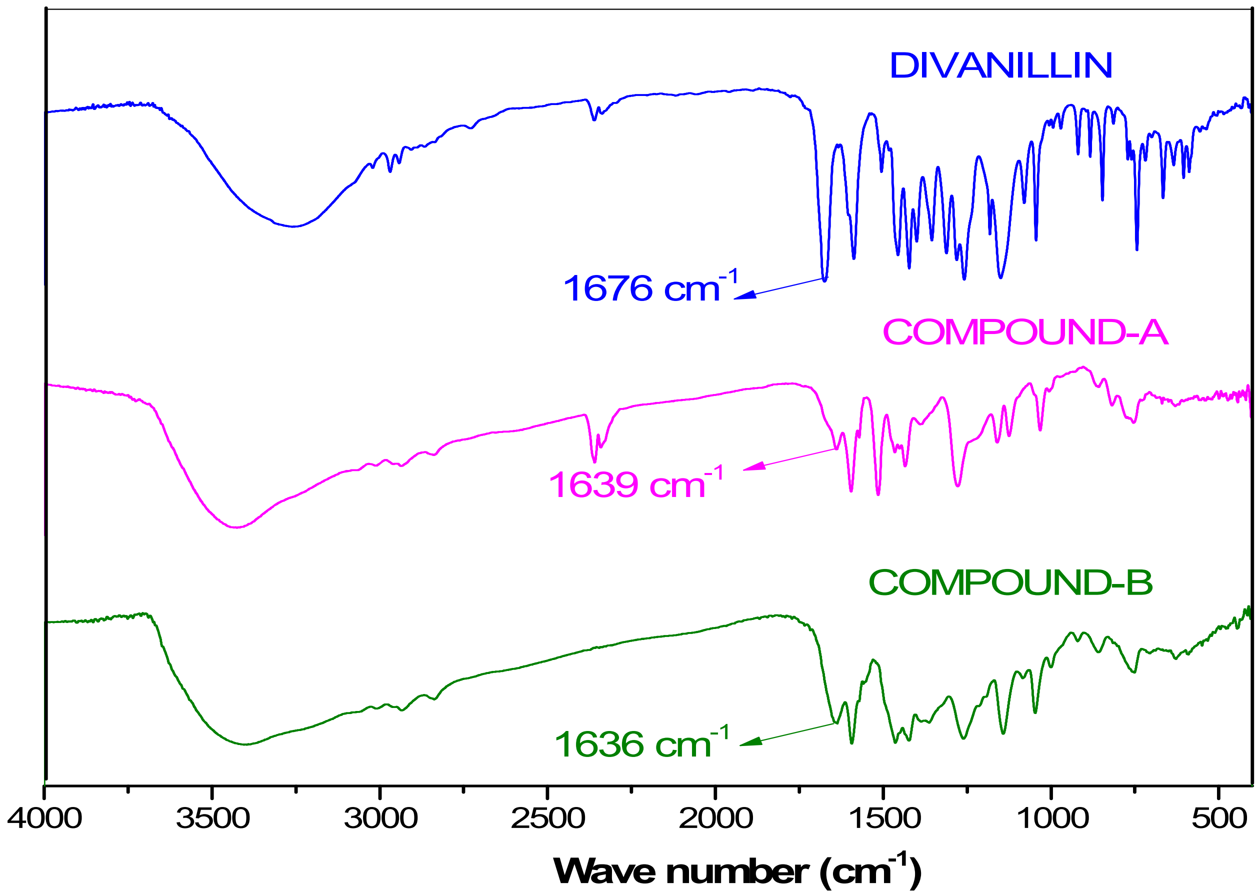


Fig. S4 FTIR spectra of divanillin, Compound A and Compound B

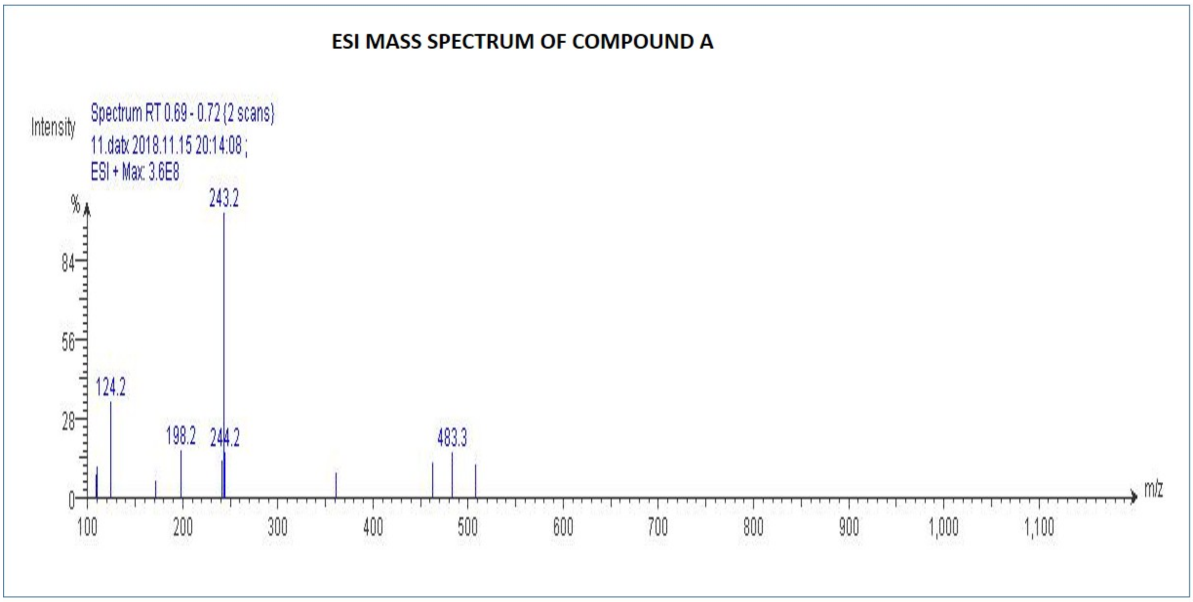


Fig. S5 ESI-Mass spectrum of Compound A

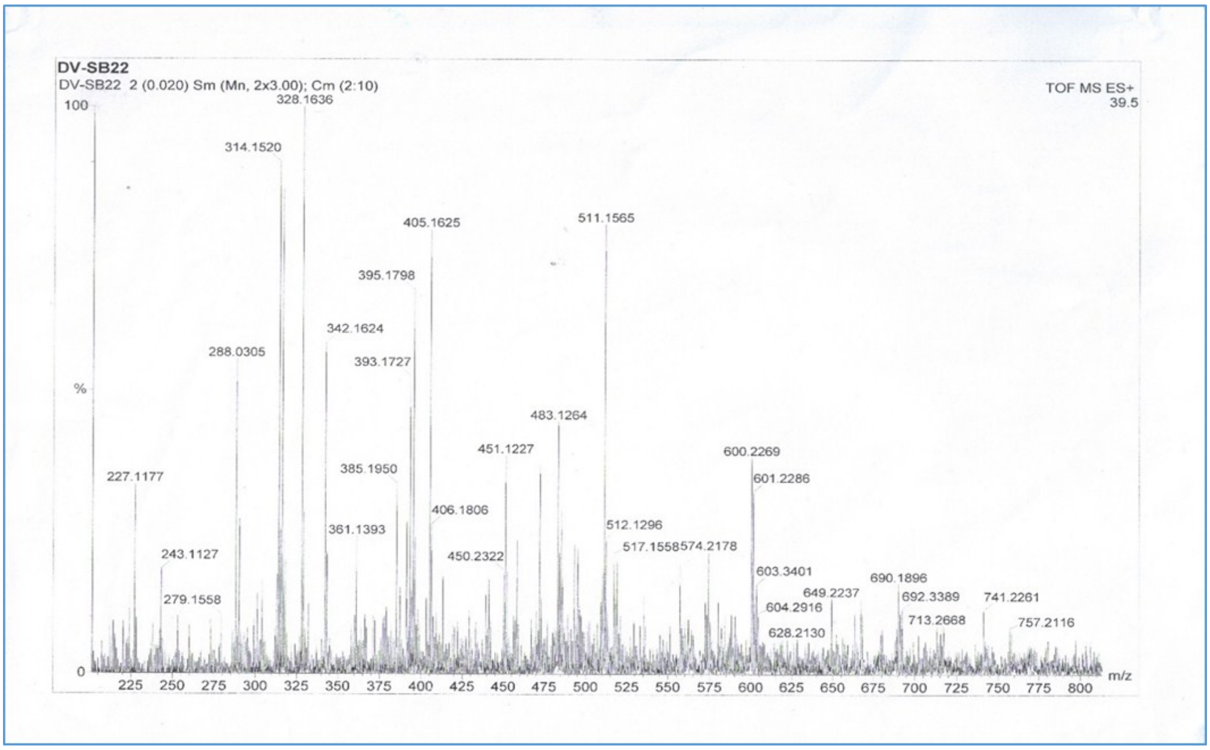


Fig. S6 ESI-Mass spectrum of Compound B

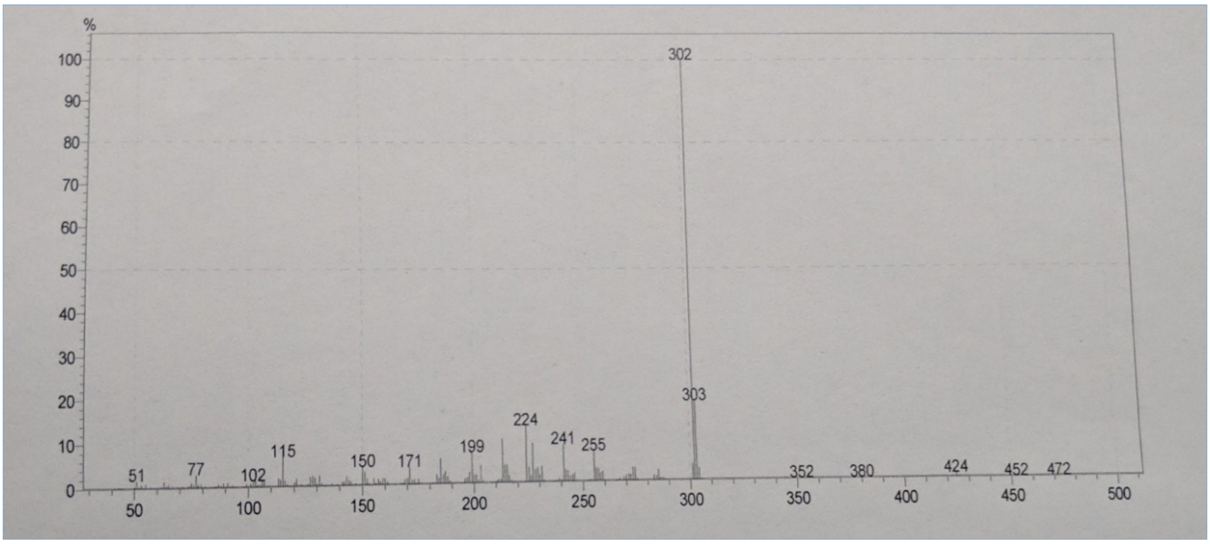


Fig. S7 EI-Mass spectrum of divanillin

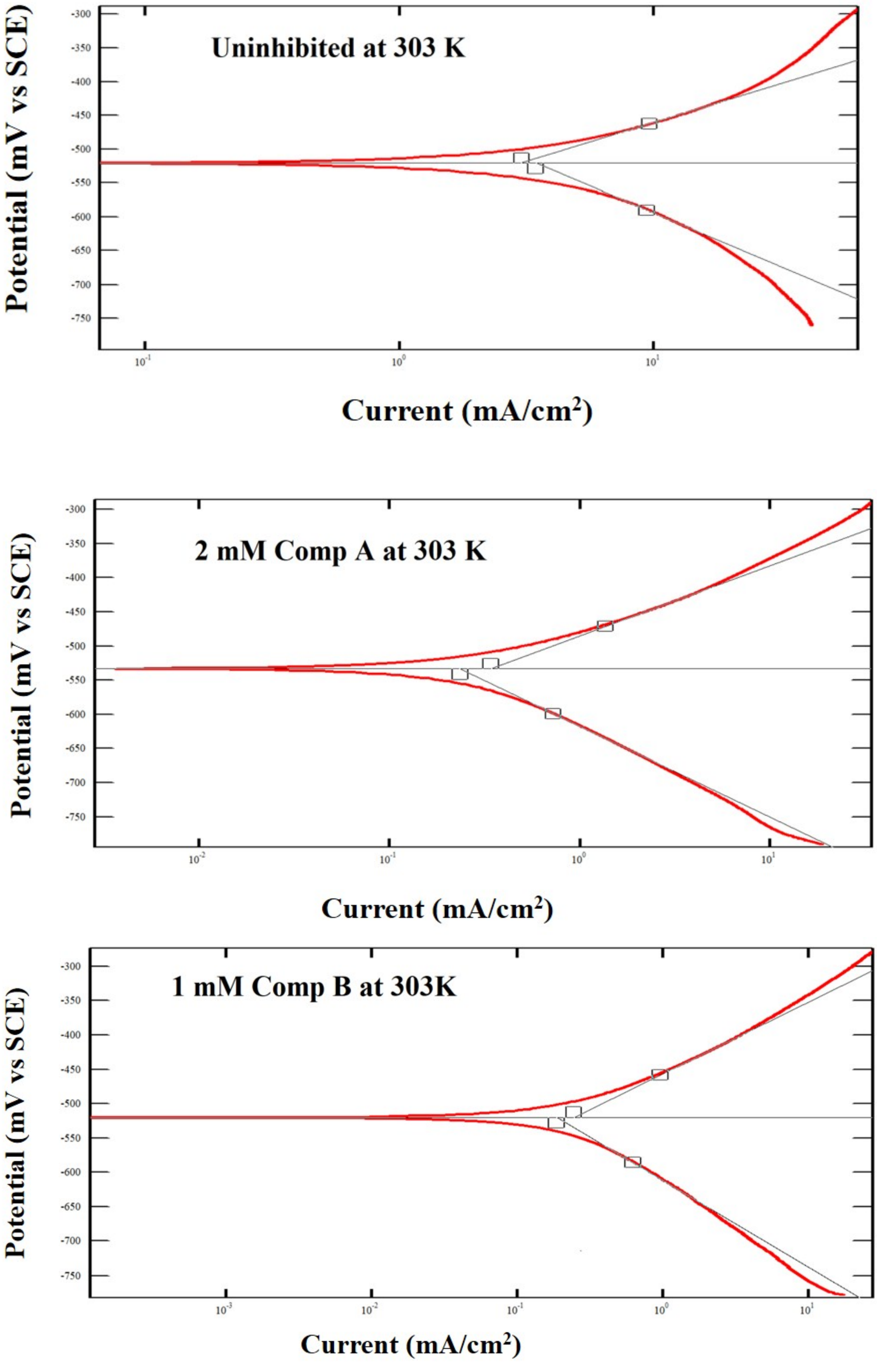


Fig. S8 Fitting of the Potentiodynamic polarization plots of uninhibited (top) and inhibited (middle and lower figures represent 1mM of Comp A and B respectively) samples at 303K.

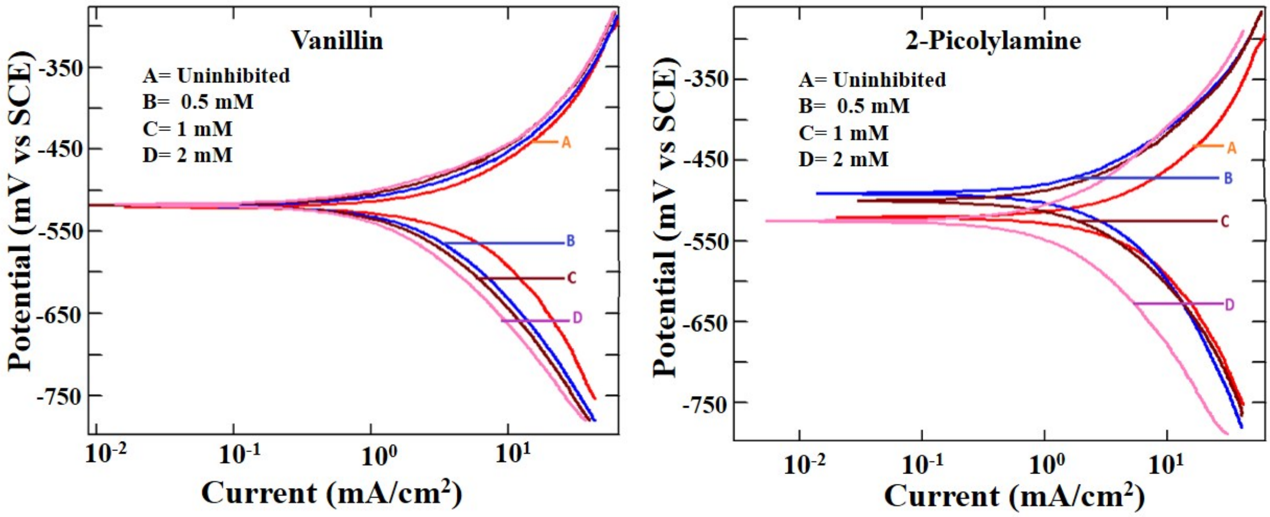


Fig. S9 Potentiodynamic polarization plots for mild steel in 1 M HCl in presence of vanillin (left) and 2-picolylamine (right) at 303K.

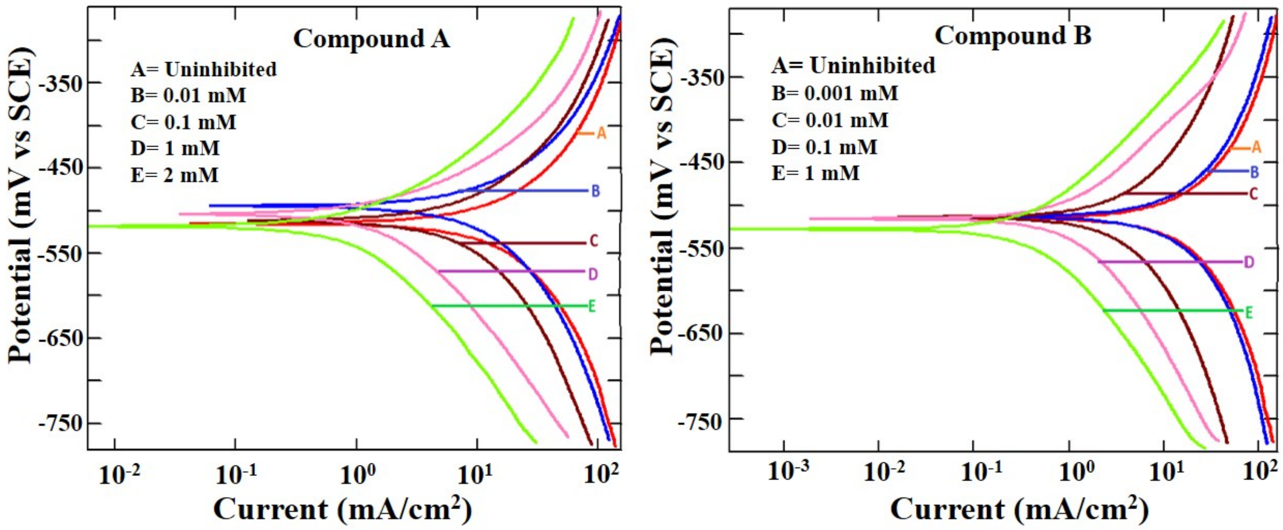


Fig. S10 Potentiodynamic polarization plots for mild steel in 1 M HCl in presence of compound A (left) and compound B (right) at 323K

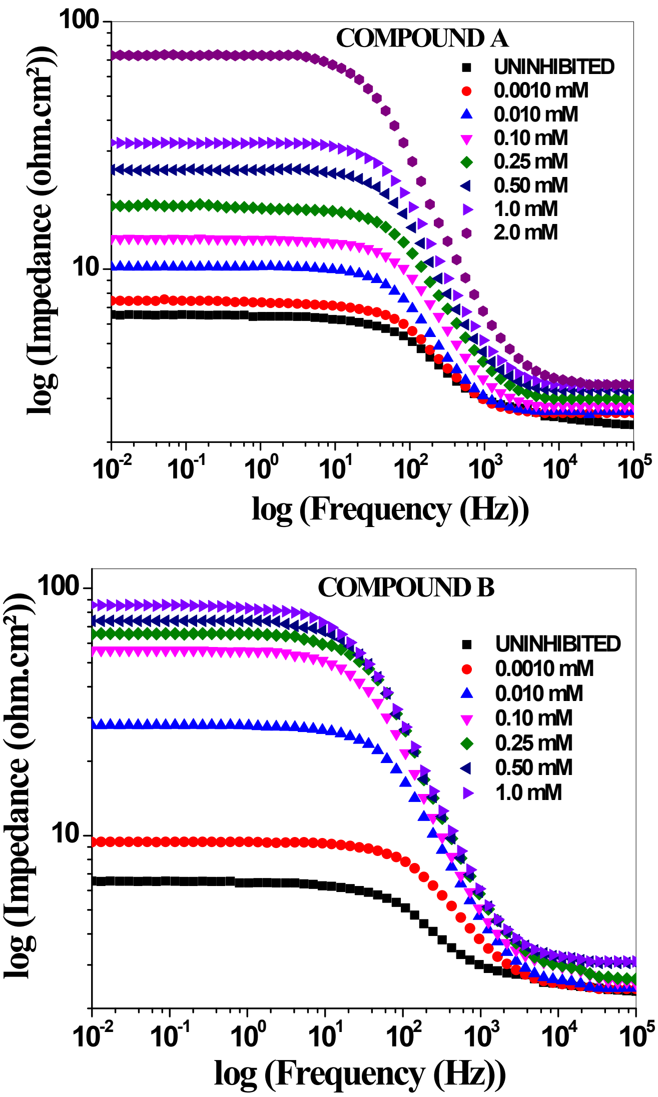
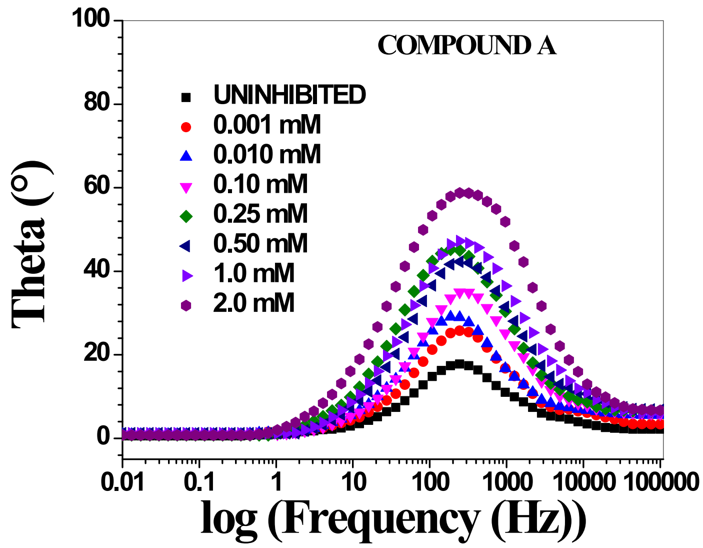


Fig. S11 Bode impedance plots in absence and presence of compound A and compound B at 303K



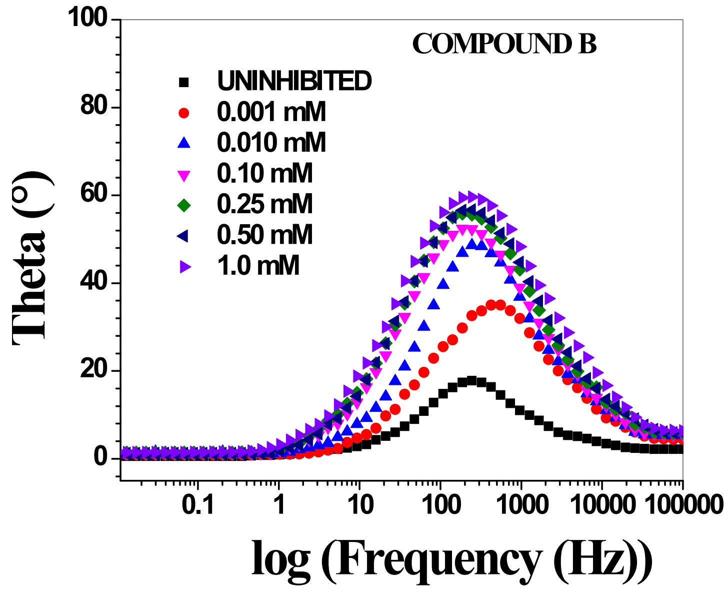


Fig. S12 Bode phase angle plots in absence and presence of compound A and compound B at 303K. Inset shows the corresponding plot for uninhibited sample.

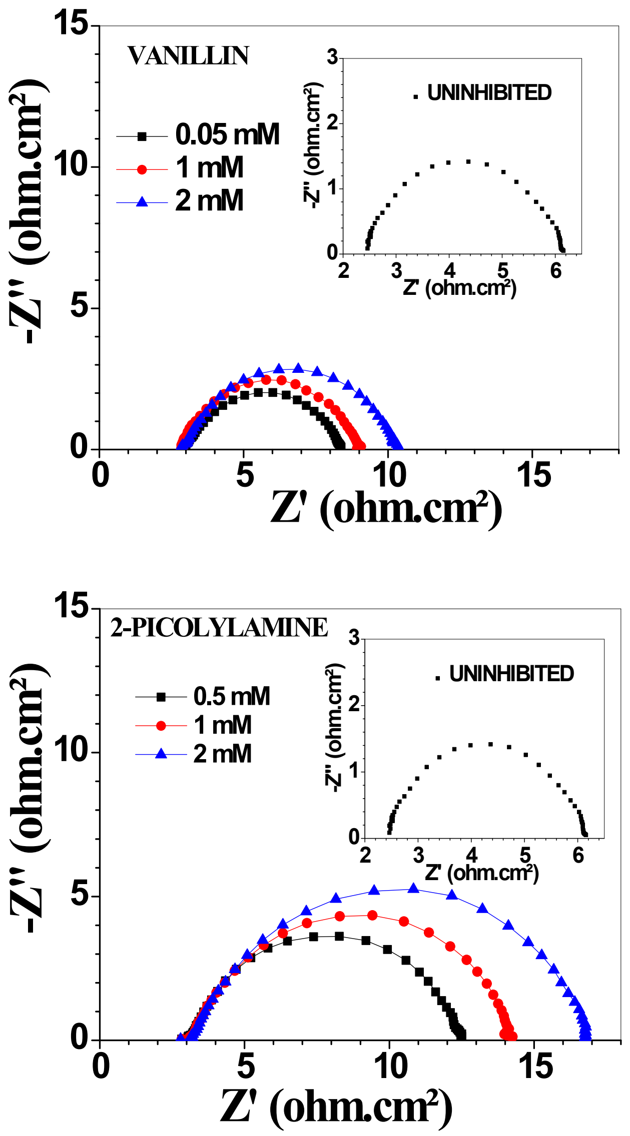


Fig. S13 Nyquist plots for mild steel in 1 M HCl in presence of vanillin (up) and 2-picolylamine (down) in 1 M HCl solution at 303K. Inset shows the corresponding plot for uninhibited sample.

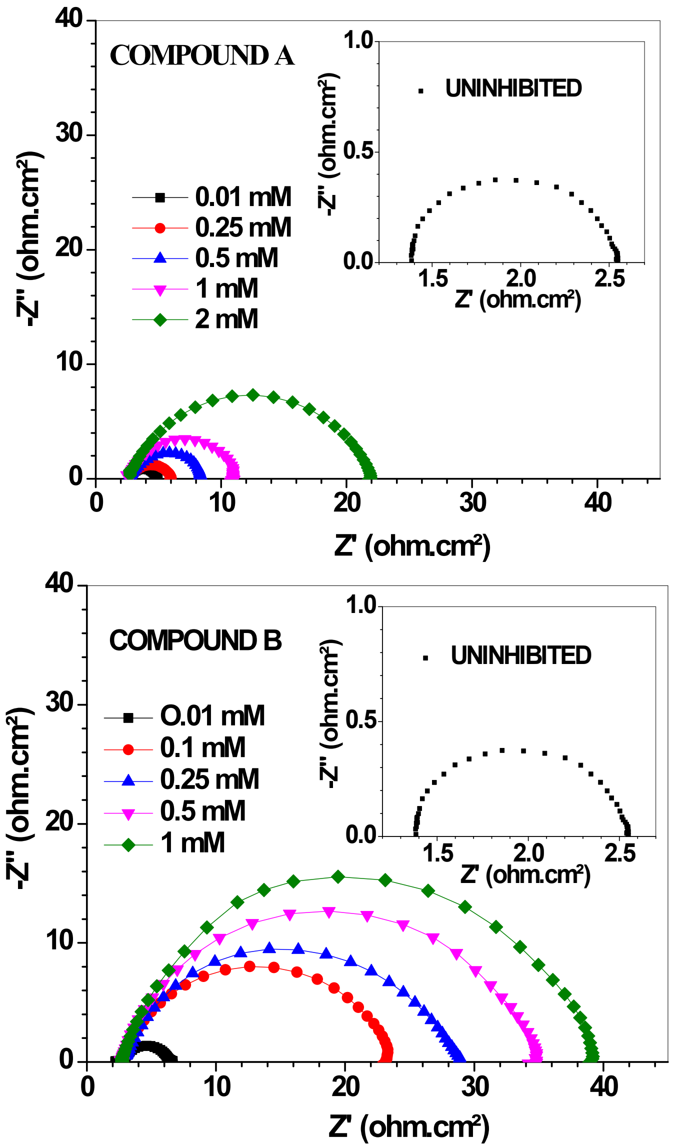


Fig. S14 Nyquist plots for mild steel in 1 M HCl in presence of compound A (up) and compound B (down) at 323K. Inset shows the corresponding plot for uninhibited sample.

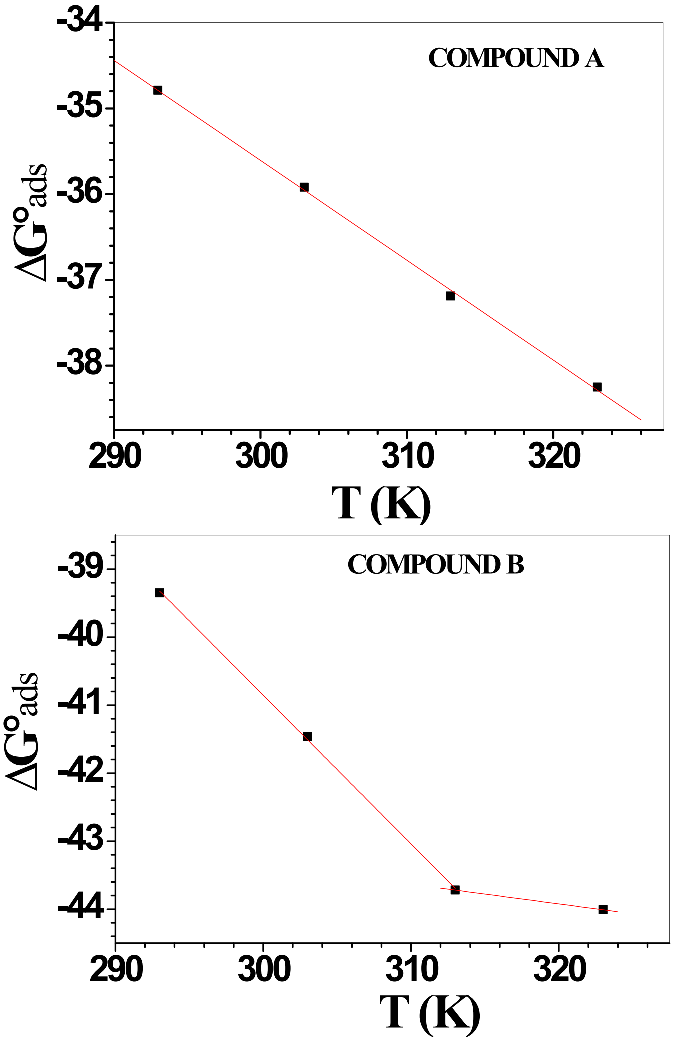
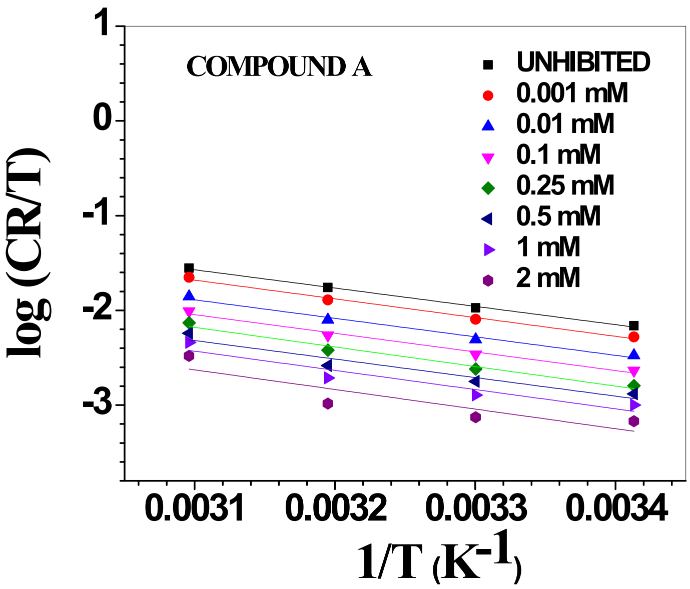


Fig. S15 Standard free energy of adsorption *vs*. Temperature plot of compound A (up) and compound B (down)



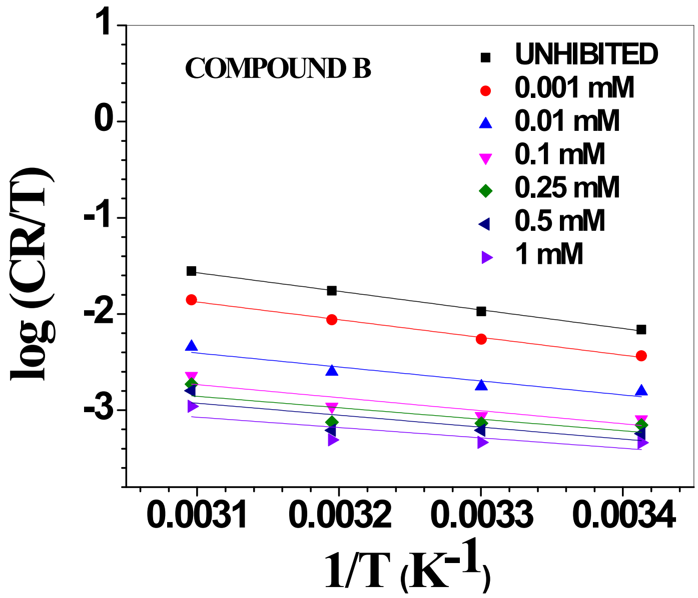


Fig. S16 Arrhenius plots for mild steel in 1 M HCl solution in absence and presence of compound A (up) and compound B (down).

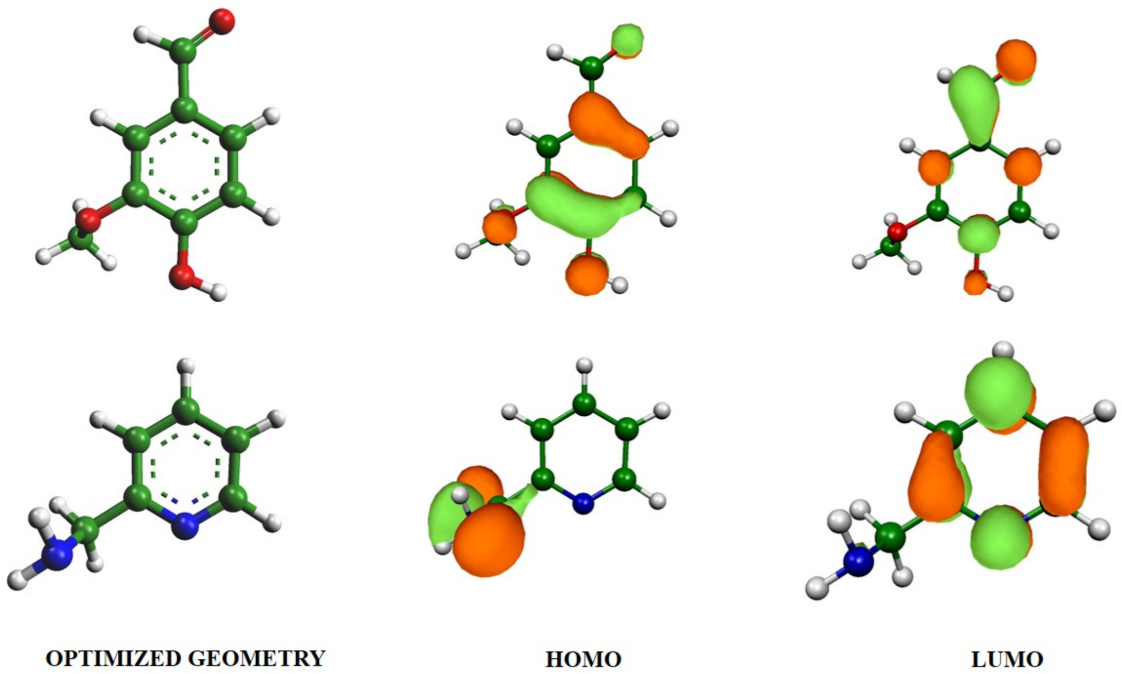


Fig. S17 Optimized geometry and electron distribution in HOMO and LUMO for vanillin (up) and 2-picolyl amine (down) as obtained from DFT study

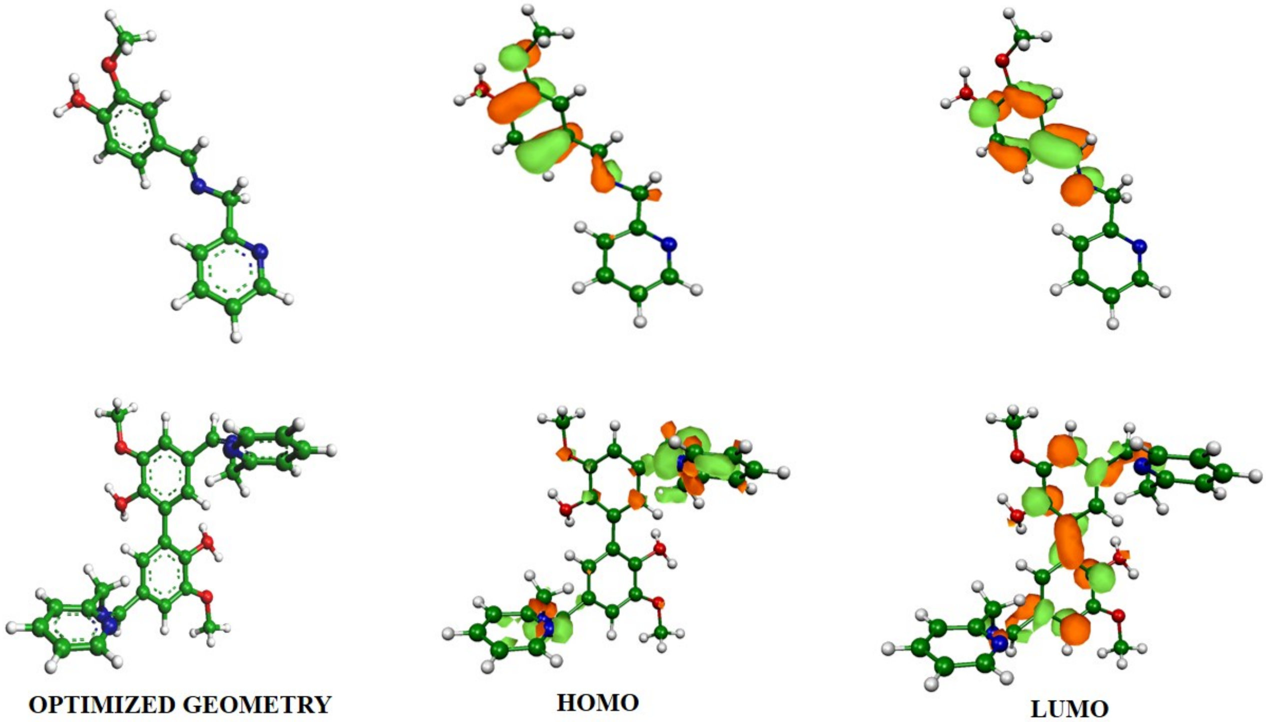


Fig. S18 Optimized geometry and electron distribution in HOMO and LUMO for compound A in monoprotonated form (up) and compound B in di-protonated form (down) as obtained from DFT study

Table S1 Potentiodynamic polarisation data for mild steel in 1 M HCl in presence of vanillin and 2-picolyl amine at 303K

Conc. of inhibitor (mM)	**-E_{corr} (mV/SCE)**	**b_a (mVdec^{-1})**	**-b_c (mVdec^{1})**	**i_{corr} (µA cm^{-2})**	**η_p%**
UNINHIBITED	521	121.4	158.7	3254	-
		vanillin			
0.001	508	105.6	133.4	2858	12.2
0.010	512	106.5	133.3	2819	13.4
0.10	507	107.7	133.1	2606	19.9
0.25	509	104.5	133.8	2337	28.2
0.50	519	107.4	135.4	2006	38.3
1.0	519	105.6	135.7	1709	47.5
2.0	512	107.1	133.4	1556	52.2
		2-picolylamine			
0.001	495	106.9	133.7	2712	16.6
0.010	506	105.8	134.1	2314	28.9
0.10	499	106.1	133.6	2133	34.5
0.25	507	106.0	134.3	1857	42.9
0.50	491	107.2	134.1	1786	45.1
1.0	499	106.6	133.5	1702	47.7
2.0	526	105.1	132.2	953	70.7

Table S2 Potentiodynamic polarisation data for mild steel in 1 M HCl in presence and absence of compound A and compound B at 323K

Conc. of inhibitor (mM)	**-E_{corr} (mV/SCE)**	**b_a (mVdec^{-1})**	**-b_c (mVdec^{-1})**	**i_{corr} (μA cm^{-2})**	**η_p%**
UNINHIBITED	513	116	147.6	11048	-
		Compound A			
0.001	496	104.3	128.5	8729	21.0
0.010	494	103.6	128.9	7592	31.3
0.10	512	104.4	125.3	5257	52.4
0.25	500	104.0	128.5	3944	64.3
0.50	501	104.3	127.5	3034	72.5
1.0	503	103.6	127.9	2062	81.3
2.0	518	105.3	128.5	990	91.0
		Compound B			
0.001	513	101.4	129.3	8301	24.9
0.010	514	103.3	129.9	2405	78.2
0.10	515	104.4	125.5	909	91.7
0.25	515	103.9	127.3	633	94.3
0.50	516	102.8	127.7	590	94.7
1.0	527	104.1	127.3	399	96.4

Table S3 EIS data for mild steel in 1 M HCl in presence of vanillin and 2-picolyl amine at 303K

Conc. of inhibitor (mM)	R_p **(Ωcm²)**	Q **(μΩ⁻¹sⁿ cm⁻²)**	n	C_{dl} **(μF cm⁻²)**	η_z**%**	$\chi^2\times10^4$
UNINHIBITED	3.8	1010	0.81	273.9		4.21
			vanillin			
0.001	3.6	1680	0.80	468.5	-	2.41
0.010	3.9	1360	0.80	367.0	2.6	3.41
0.10	4.2	970	0.81	266.8	9.5	3.04
0.25	4.6	819	0.81	221.2	17.4	2.34
0.50	5.3	727	0.81	197.4	28.3	2.444
1.0	6.3	667	0.81	184.8	39.7	3.27
2.0	7.6	626	0.82	193.5	50.0	2.98
			2-picolylamine			
0.001	3.8	687	0.82	186.2	-	2.77
0.010	4.2	665	0.82	182.9	9.5	2.99
0.10	6.2	632	0.82	187.2	38.7	3.23
0.25	7.8	525	0.82	157.0	51.3	2.62
0.50	9.3	422	0.83	135.7	59.1	2.61
1.0	11.1	353	0.83	113.5	65.8	3.52
2.0	13.7	313	0.83	102.5	72.3	3.17

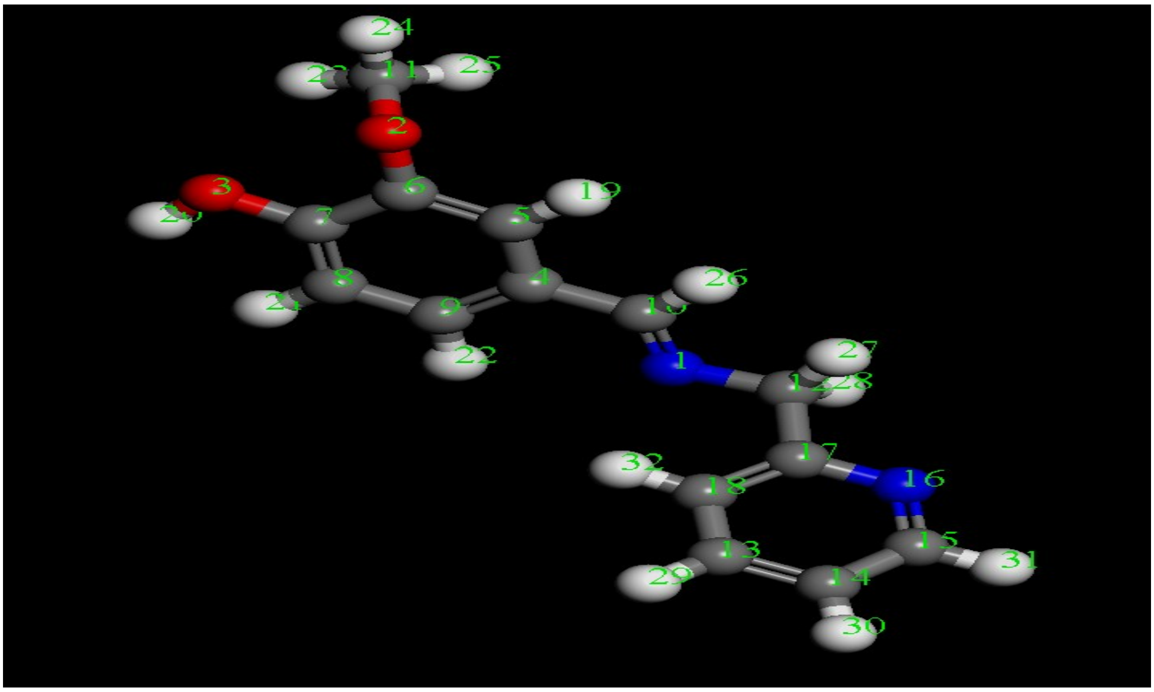
Table S4 EIS data for mild steel in 1 M HCl in presence and absence of Compound A and compound B at 323K

Conc. of inhibitor (mM)	R_p **(Ωcm^2)**	Q **(μΩ^{-1}s^n cm^{-2})**	n	C_{dl} **(μF cm^{-2})**	η_z**%**	**χ^2×10^4**
UNINHIBITED	1.2	1980	0.82	525.6	-	0.51
			Compound A			
0.001	1.3	3000	0.85	1127.2	7.7	0.44
0.010	1.6	2014	0.85	731.7	25.0	0.47
0.10	2.3	817	0.85	269.9	47.8	3.2
0.25	3.4	769	0.85	269.3	64.7	1.22
0.50	5.8	361	0.85	121.5	79.3	1.01
1.0	8.5	322	0.86	123.2	85.9	2.69
2.0	19.4	216	0.86	88.6	93.8	2.17
			Compound B			
0.001	1.6	1680	0.82	458.2	33.3	0.61
0.010	3.6	1280	0.83	425.3	66.7	2.81
0.10	21.0	277	0.83	96.5	94.3	.64
0.25	25.4	256	0.85	105.3	95.3	1.59
0.50	31	168	0.86	71.4	96.1	0.69
1.0	36.9	157	0.86	67.9	96.8	0.86

Table S5 Corrosion rate of mild steel in 1 M HCl in presence and absence of 1 mM compound A and compound B at different exposure times at 303K

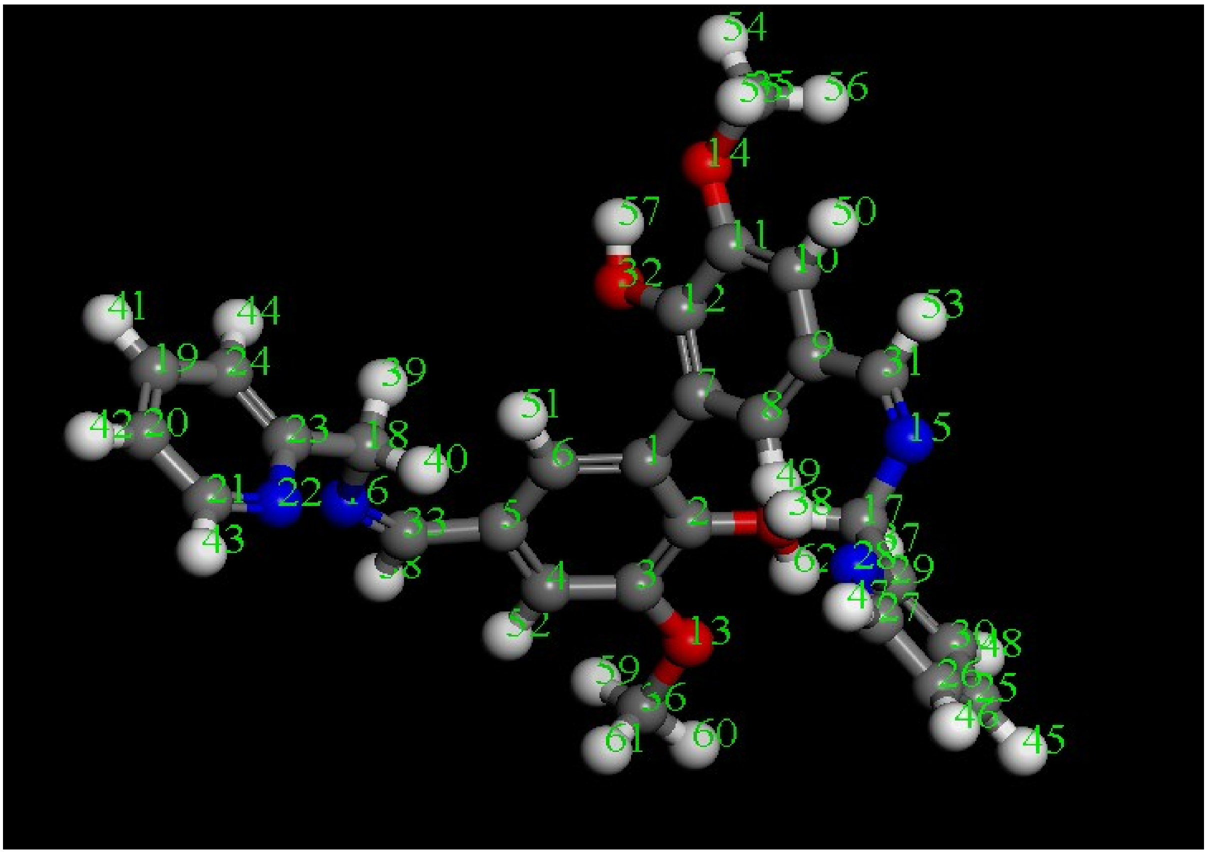
Exposure Time (h)	**Inhibitor**	**Weight loss (mg)**	**Corrosion Rate (mg cm^{-2} h^{-1})**	**η_W%**
6	Uninhibited	259.8	3.207	-
	Compound A	31.3	0.386	88.0
	Compound B	11.3	0.140	95.6
24	Uninhibited	1210.3	3.735	-
	Compound A	142.8	0.441	88.2
	Compound B	49.6	0.153	95.9
48	Uninhibited	1796.7	2.773	-
	Compound A	262.3	0.405	85.4
	Compound B	116.8	0.180	93.5
72	Uninhibited	2141.5	2.203	-
	Compound A	359.8	0.370	83.2
	Compound B	192.7	0.198	91.0
96	Uninhibited	2453.7	1.893	-
	Compound A	505.5	0.390	79.4
	Compound B	282.2	0.217	88.5

Table S6. Calculated Fukui functions of the atoms present in compound A, compound B, vanillin and 2-picolyl amine respectively with their numbering of theirs atoms.



Compound A		
atom	f_k^+	f_k^-
N (1)	0.109	0.073
O (2)	0.017	0.047
O (3)	0.047	0.103
C (4)	0.053	0.085
C (5)	0.055	0.046
C (6)	0.035	0.068
C (7)	0.067	0.081
C (8)	0.042	0.057
C (9)	0.070	0.067
C (10)	0.120	0.040

C (11)	0.008	0.017
C (12)	0.023	0.018
C (13)	0.021	0.007
C (14)	0.016	0.009
C (15)	0.017	0.009
N (16)	0.022	0.015
C (17)	0.012	0.006
C (18)	0.013	0.007
H (19)	0.028	0.028
H (20)	0.019	0.036
H (21)	0.023	0.030
H (22)	0.034	0.031
H (23)	0.006	0.073
H (24)	0.007	0.047
H (25)	0.007	0.103
H (26)	0.048	0.085
H (27)	0.020	0.046
H (28)	0.028	0.068
H (29)	0.010	0.081
H (30)	0.008	0.057
H (31)	0.009	0.067
H (32)	0.010	0.040

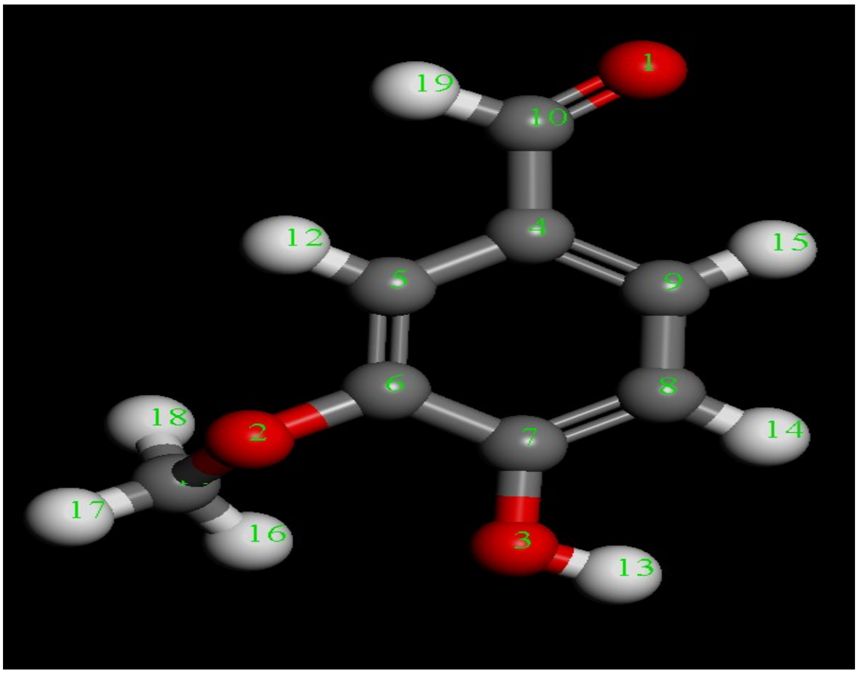


Compound B		
atom	f_k^+	f_k^-
C (1)	0.015	0.022
C (2)	0.036	0.042
C (3)	0.019	0.037
C (4)	0.033	0.028
C (5)	0.028	0.040
C (6)	0.028	0.035
C (7)	0.016	0.021
C (8)	0.028	0.035
C (9)	0.028	0.040
C (10)	0.034	0.027

C (11)	0.019	0.036
C (12)	0.037	0.041
O (13)	0.011	0.039
O (14)	0.011	0.039
N (15)	0.063	0.042
N (16)	0.062	0.043
C (17)	0.011	0.007
C (18)	0.011	0.007
C (19)	0.010	0.003
C (20)	0.008	0.003
C (21)	0.009	0.003
N (22)	0.009	0.004
C (23)	0.004	0.001
C (24)	0.008	0.002
C (25)	0.010	0.002
C (26)	0.008	0.003
C (27)	0.009	0.003
N (28)	0.010	0.004
C (29)	0.004	0.001
C (30)	0.008	0.002
C (31)	0.058	0.019
O (32)	0.027	0.051
C (33)	0.058	0.019
O (34)	0.027	0.051
C (35)	0.005	0.011

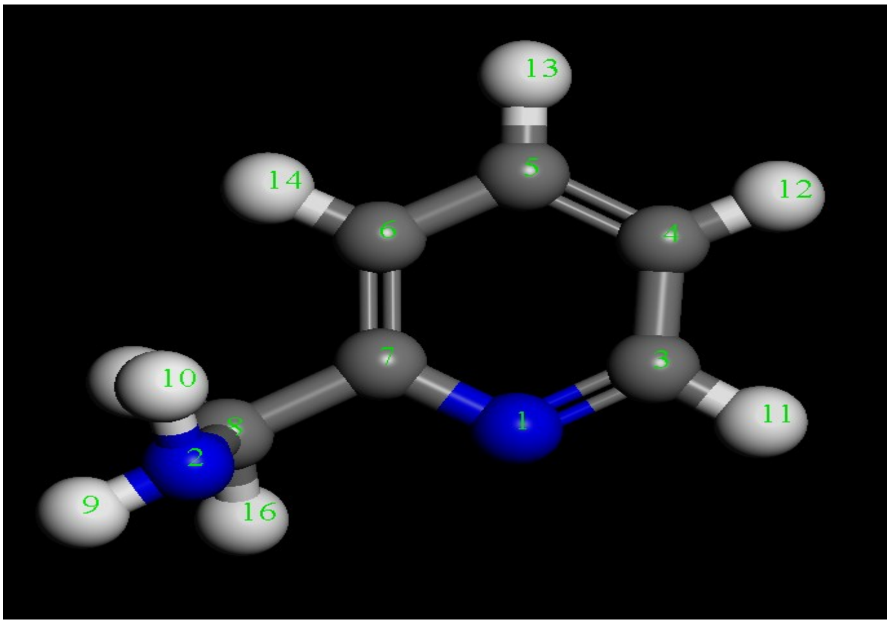
C (36)	0.005	0.011
H (37)	0.013	0.009
H (38)	0.012	0.008
H (39)	0.014	0.009
H (40)	0.011	0.008
H (41)	0.005	0.002
H (42)	0.004	0.002
H (43)	0.004	0.002
H (44)	0.005	0.002
H (45)	0.005	0.002
H (46)	0.004	0.002
H (47)	0.004	0.002
H (48)	0.005	0.002
H (49)	0.012	0.015
H (50)	0.015	0.015
H (51)	0.012	0.015
H (52)	0.015	0.015
H (53)	0.023	0.013
H (54)	0.004	0.008
H (55)	0.004	0.010
H (56)	0.004	0.010
H (57)	0.011	0.019
H (58)	0.023	0.013
H (59)	0.004	0.010
H (60)	0.004	0.008

H (61)	0.004	0.010
H (62)	0.011	0.019



vanilin		
atom	$\boldsymbol{f_k^+}$	$\boldsymbol{f_k^-}$
O (1)	0.173	0.143
O (2)	0.019	0.064
O (3)	0.058	0.097
C (4)	0.052	0.081
C (5)	0.066	0.048
C (6)	0.037	0.074
C (7)	0.078	0.074
C (8)	0.047	0.053

C (9)	0.078	0.064
C (10)	0.175	0.062
C (11)	0.008	0.020
H (12)	0.033	0.030
H (13)	0.023	0.034
H (14)	0.026	0.030
H (15)	0.037	0.033
H (16)	0.006	0.014
H (17)	0.008	0.015
H (18)	0.008	0.018
H (19)	0.067	0.048

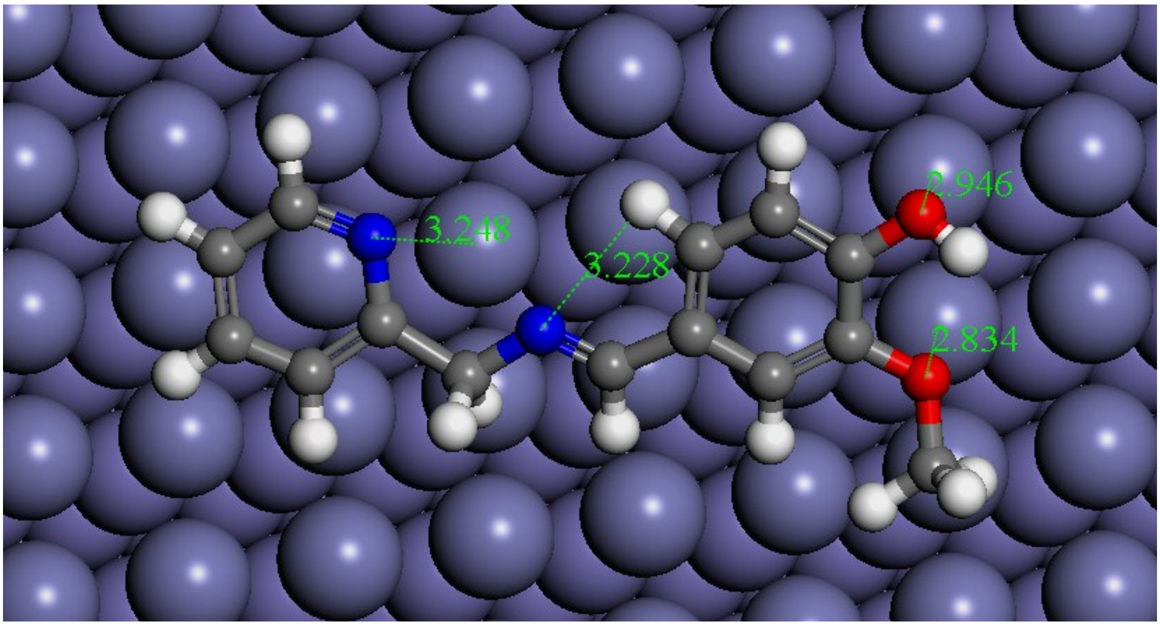


2-picolyl amine

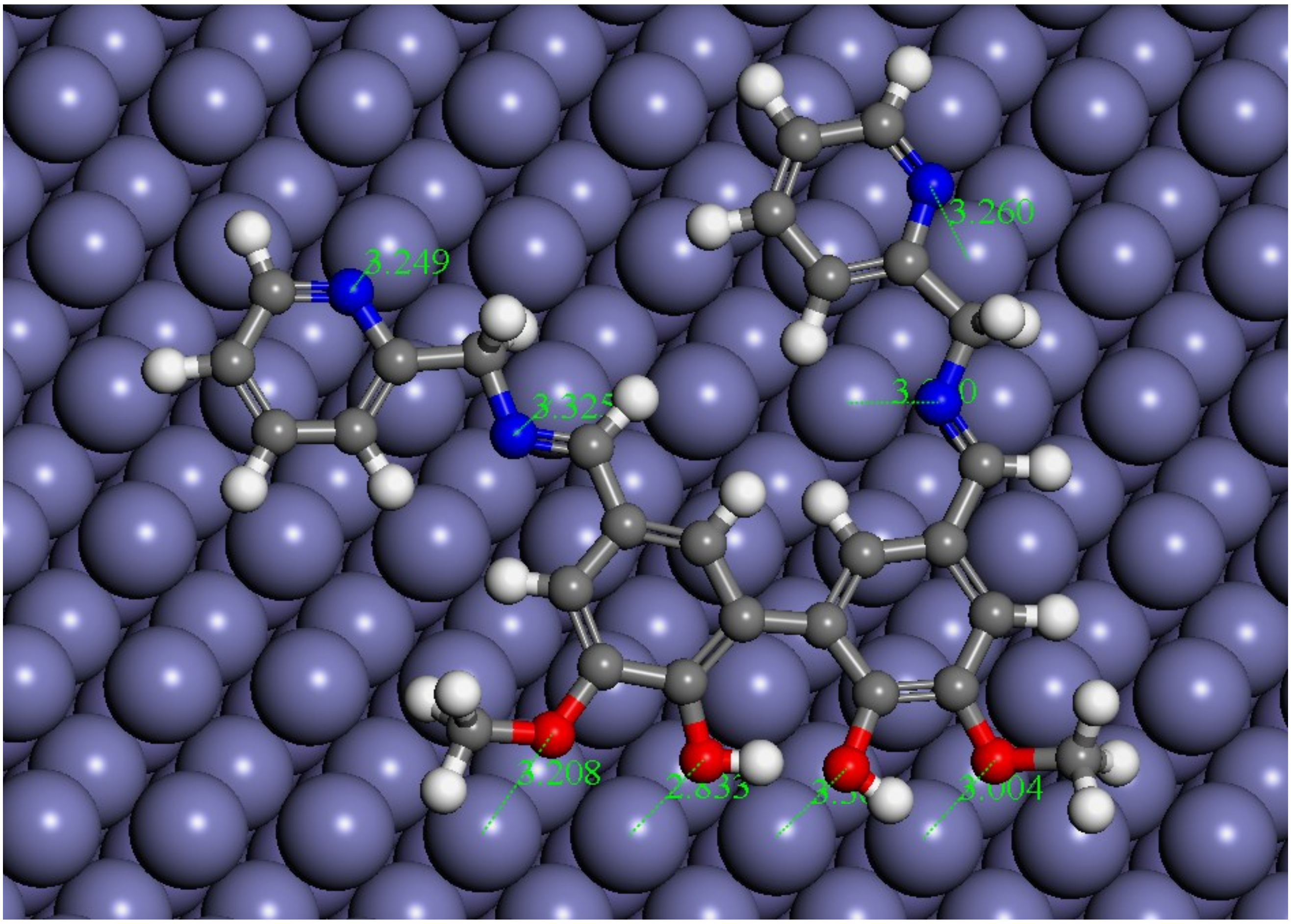
atom	f_k^+	f_k^-
N (1)	0.153	0.086

N (2)	0.020	0.328
C (3)	0.103	0.035
C (4)	0.097	0.032
C (5)	0.156	0.028
C (6)	0.082	0.028
C (7)	0.088	0.017
C (8)	0.022	0.060
H (9)	0.018	0.094
H (10)	0.013	0.091
H (11)	0.049	0.023
H (12)	0.047	0.018
H (13)	0.065	0.017
H (14)	0.043	0.019
H (15)	0.020	0.082
H (16)	0.025	0.043

Table S7 Closest distance of mild steel surface and atoms of compound A and compound B as obtained from MD simulation study



Compound A	
Fe- Atom	Closest distance
Fe- N (1)	3.228
Fe- O (2)	2.834
Fe- O (3)	2.946
Fe- N (16)	3.248



Compound B	
Fe- Atom	Closest distance
Fe- O (32)	3.369
Fe- O (14)	3.004
Fe- O (13)	3.208
Fe- O (34)	2.833
Fe- N (15)	3.080
Fe- N (28)	3.260
Fe- N (16)	3.325
Fe- N (22)	3.249