Supporting Information

Tunable Anticorrosive Effects of Newly Synthesized Benzothiazole Azo Dyes by Potassium Iodide Synergism for Carbon Steel in 1 M HCl: Combined Experimental and Theoretical Studies

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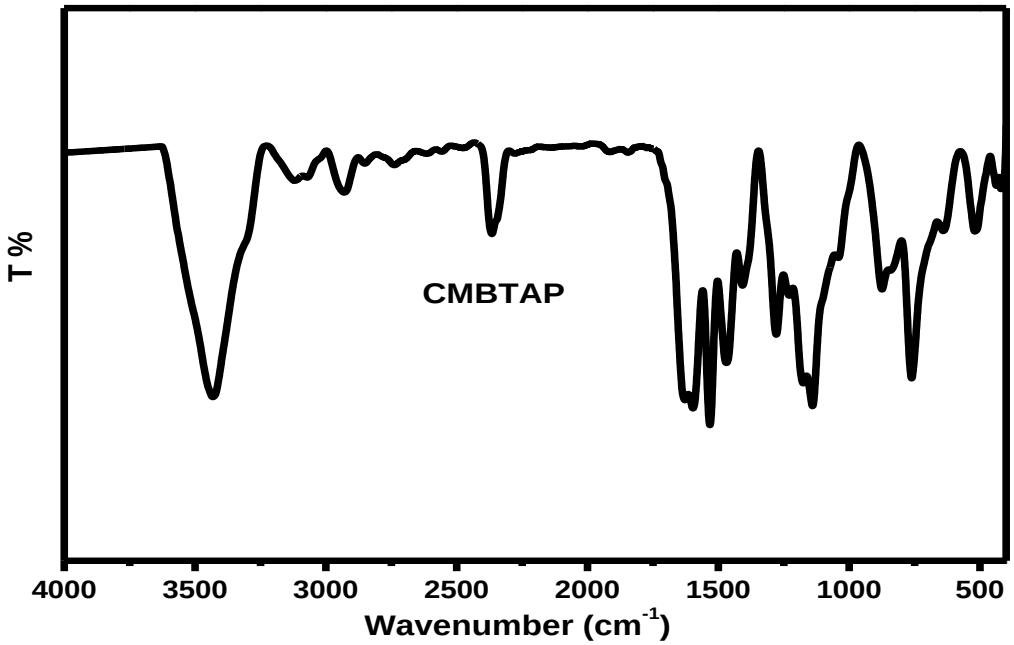


Figure S1. FT-IR spectra of the investigated CMPTAP.

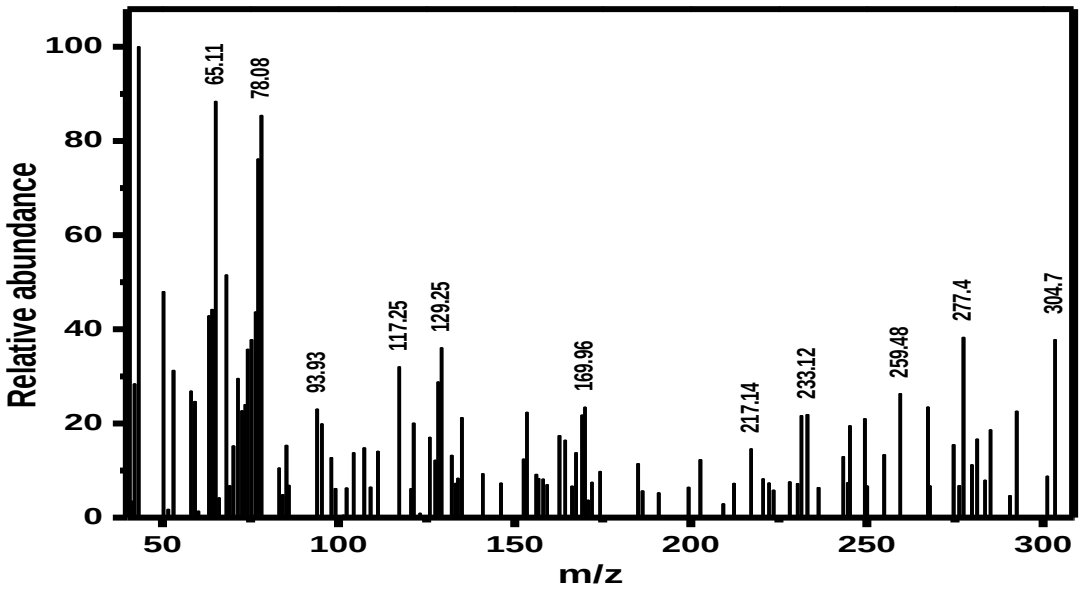


Figure S2. Mass spectrum of the investigated CMPTAP.

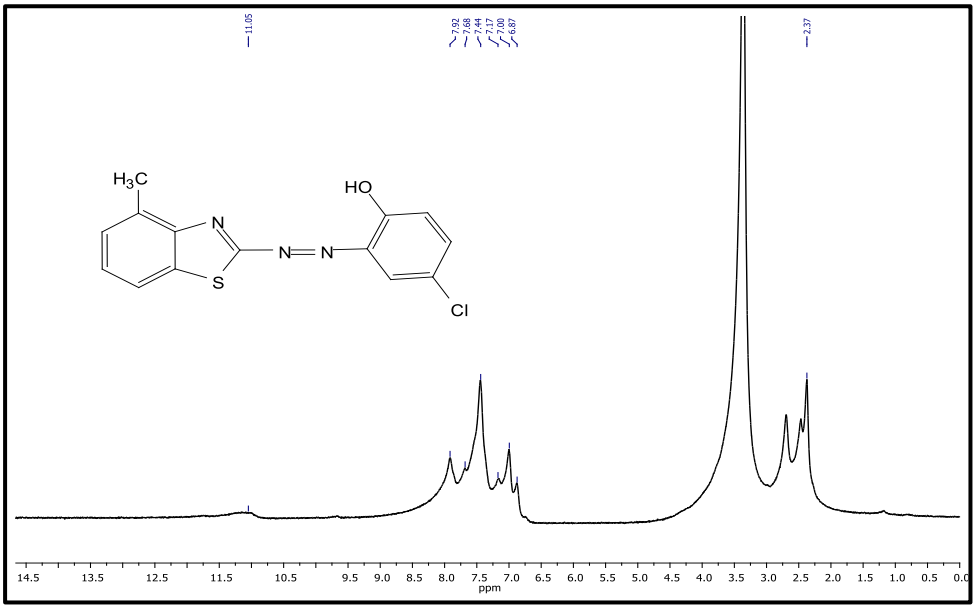


Figure S3. ^{1}H-NMR spectrum of the investigated CMPTAP in DMSO-d_6.

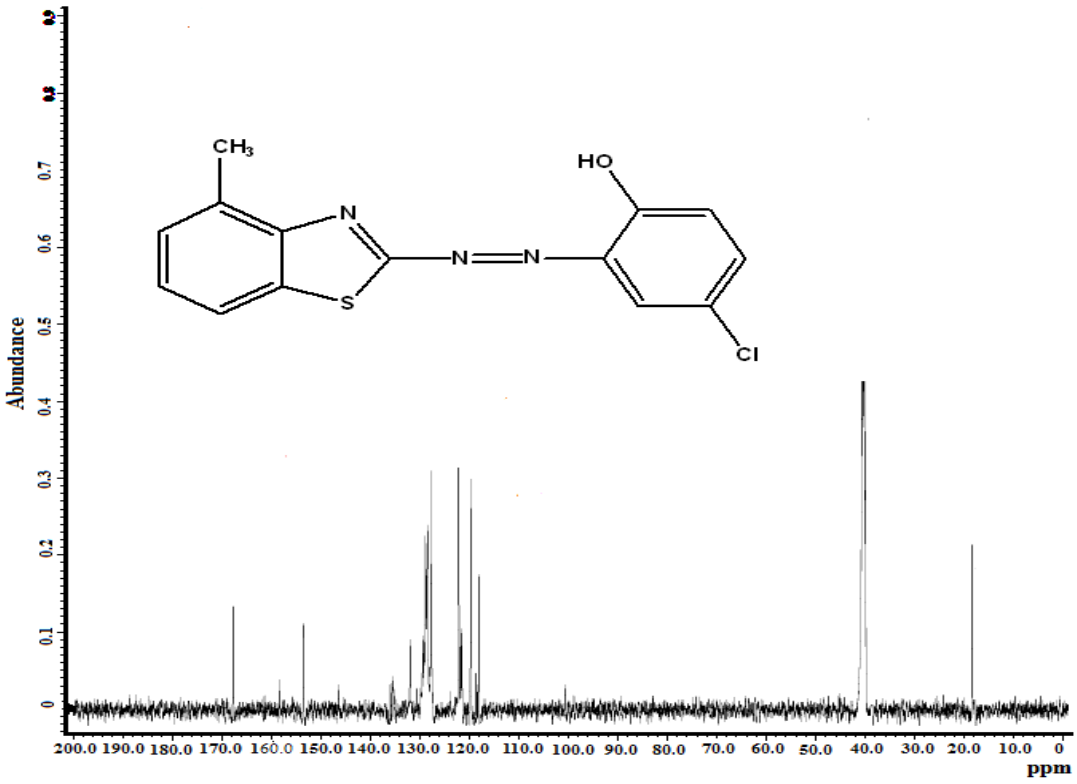


Figure S4. ^{13}C-NMR spectrum of the investigated CMPTAP in DMSO-d_6.

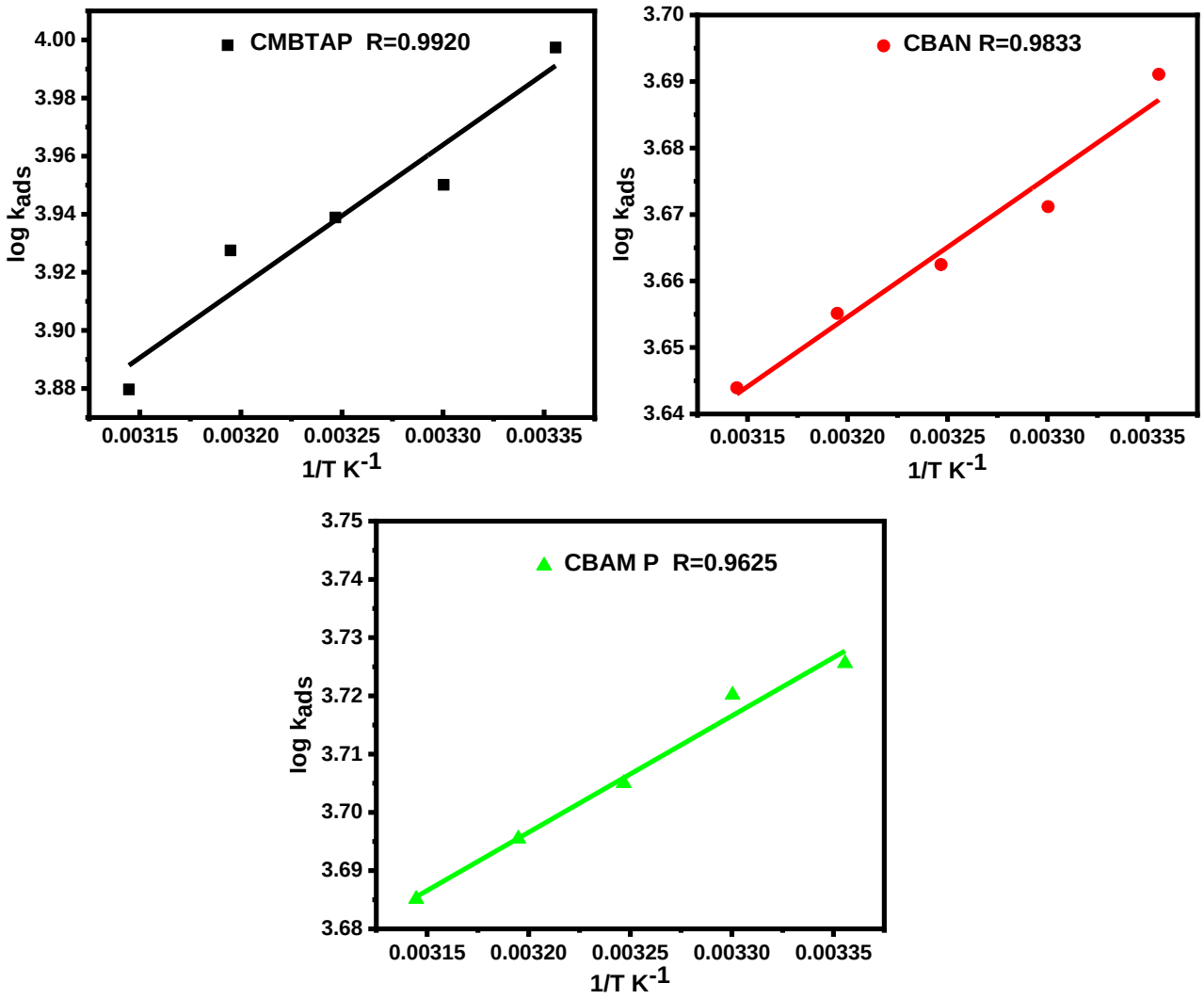


Figure S5. Log K_{ads} vs. (1/T) curves for carbon steel dissolution in 1.0 M HCl in the presence of CMBTAP, CBAN and CBAMP.

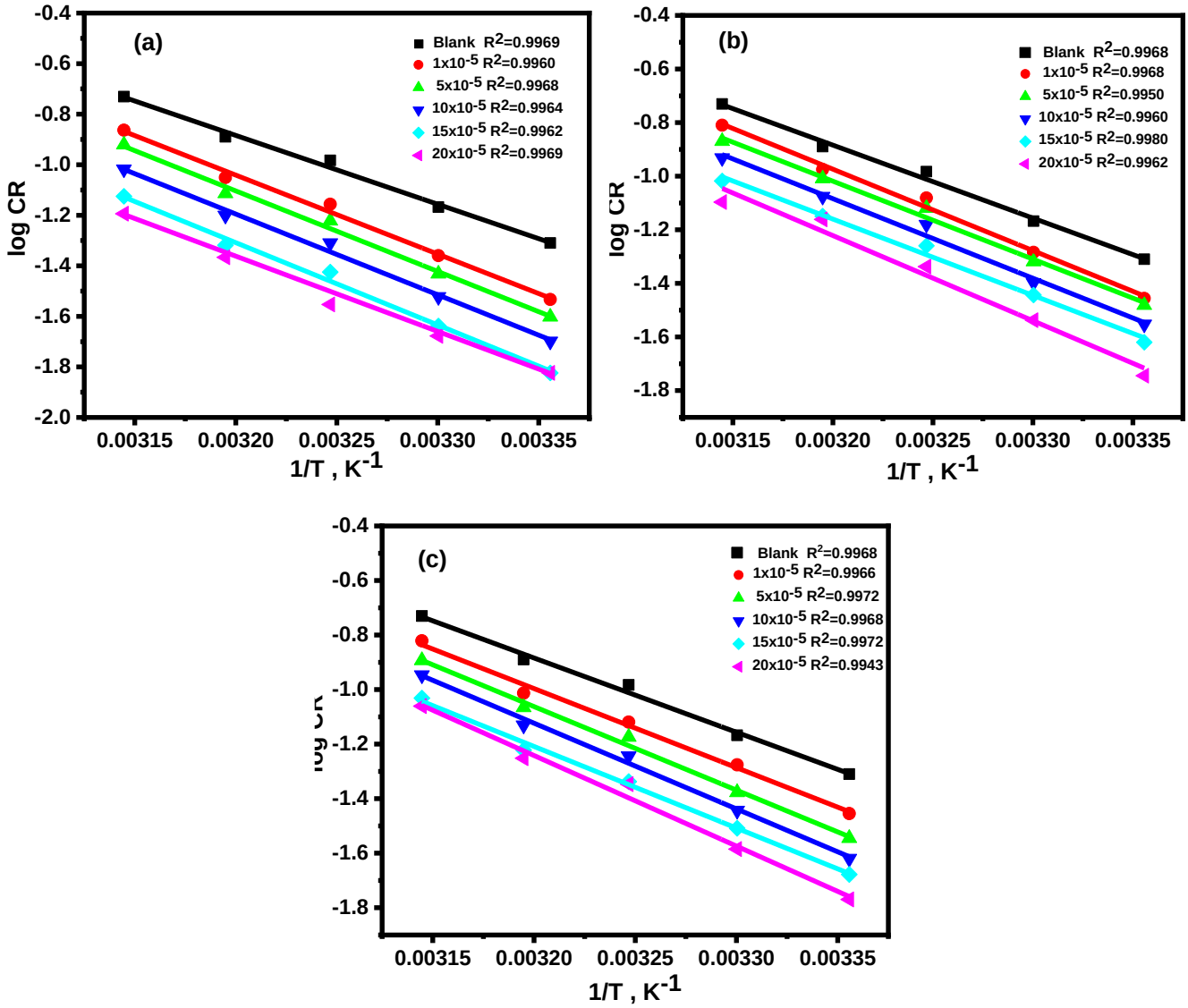


Figure S6. Arrhenius plots for carbon steel corrosion rates ($k_{corr.}$) after 120 minutes of immersion in 1.0 M HCl in the absence and presence of different concentrations of (a) CMBTAP, (b) CBAN and (c) CBAMP.

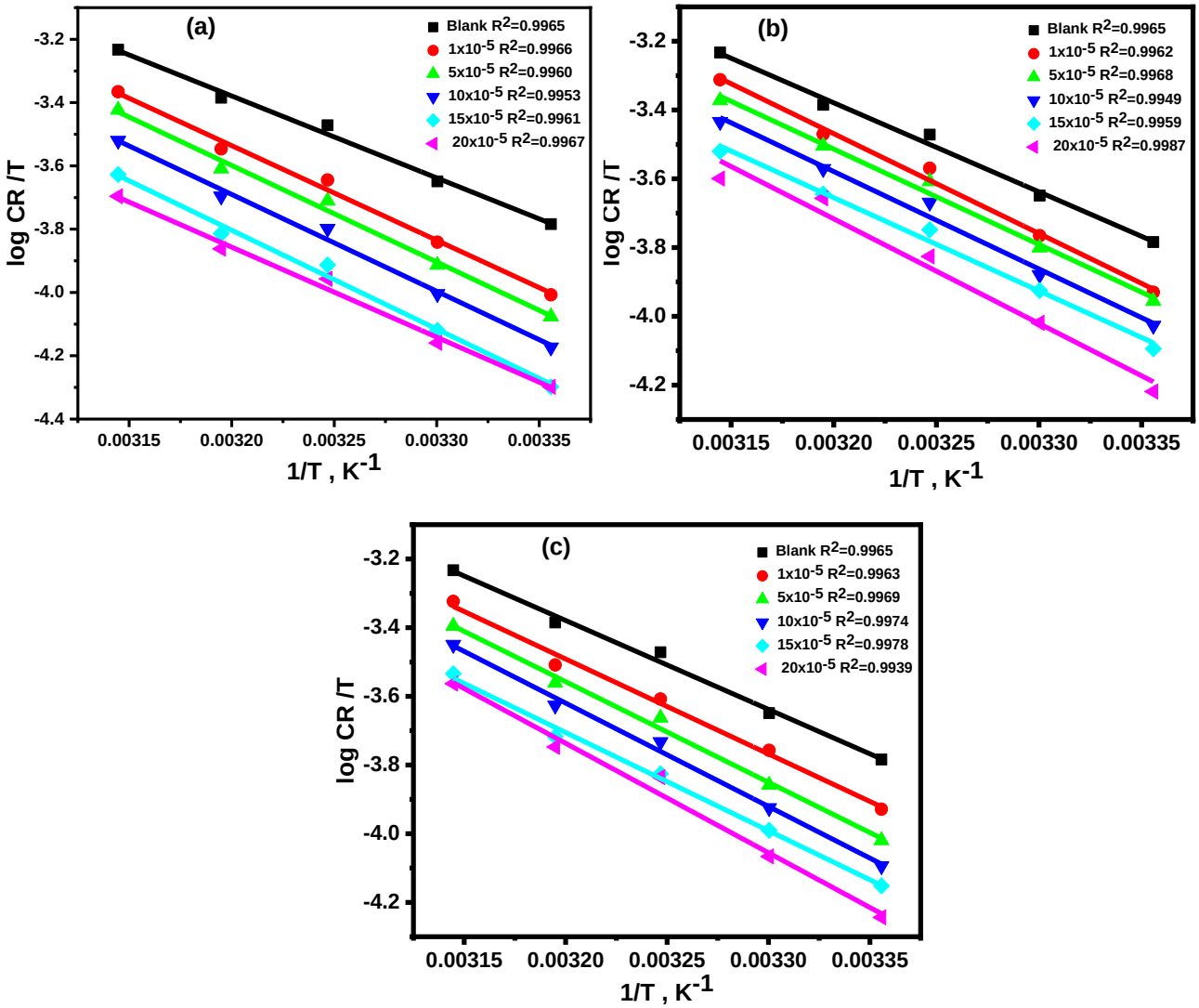


Figure S7. Plots of (log k_{corr}) vs.1/T for corrosion of C-steel in 1.0 M HCl in the absence and presence of different concentrations of (a) CMBTAP, (b) CBAN and (c) CBAMP.

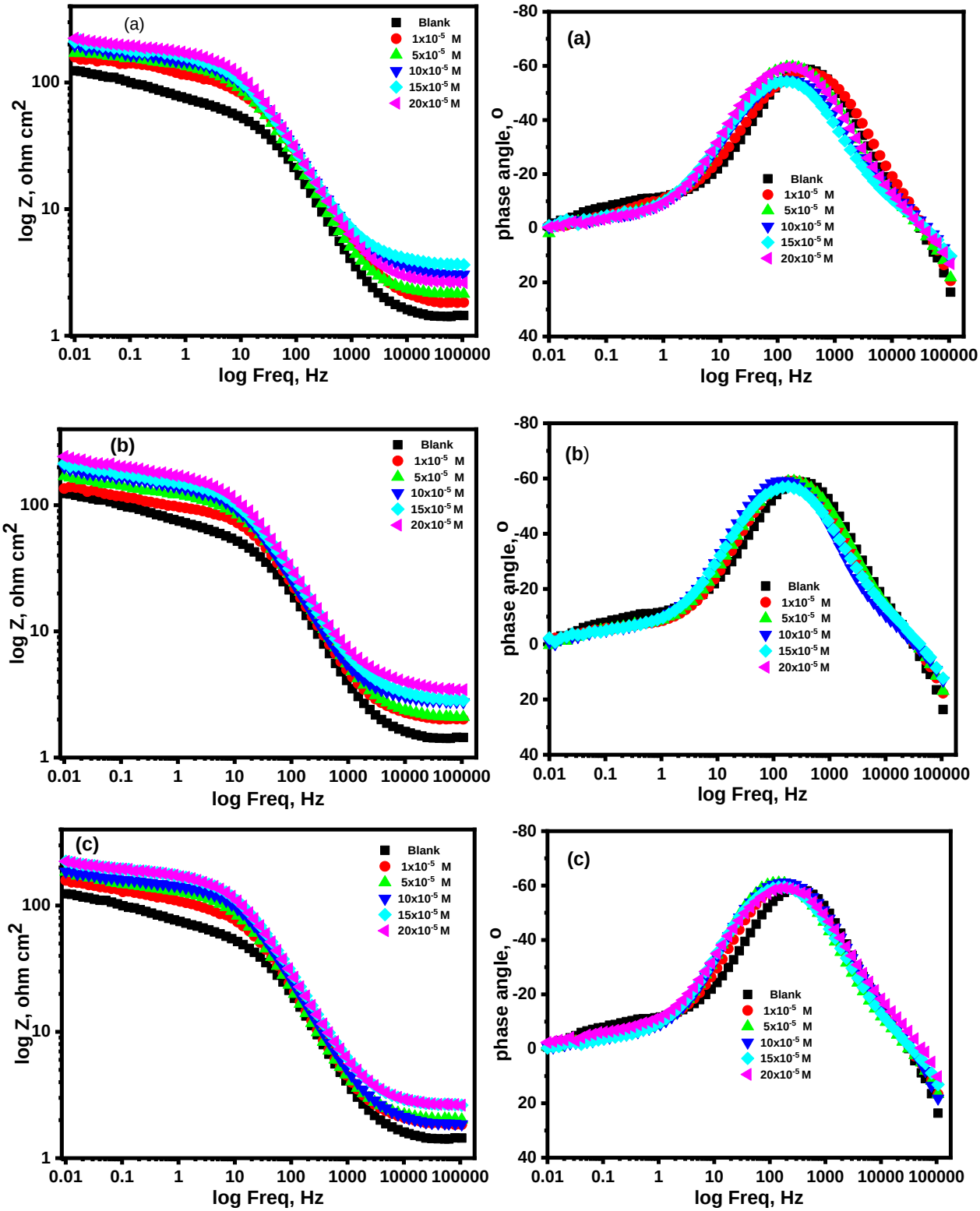


Figure S8. The Bode plots for corrosion of C-steel in 1.0 M HCl in the absence and presence of different concentrations of (a) CMBTAP, (b) CBAN and (c) CBAMP at 25°C.

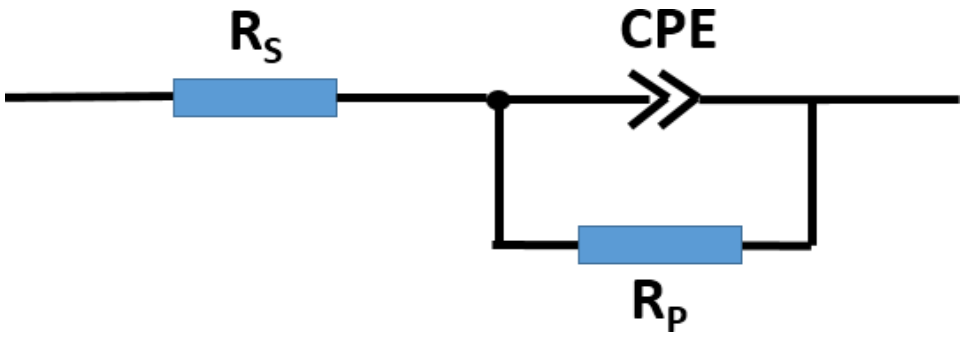


Figure S9. Equivalent circuit model used to fit experimental EIS.

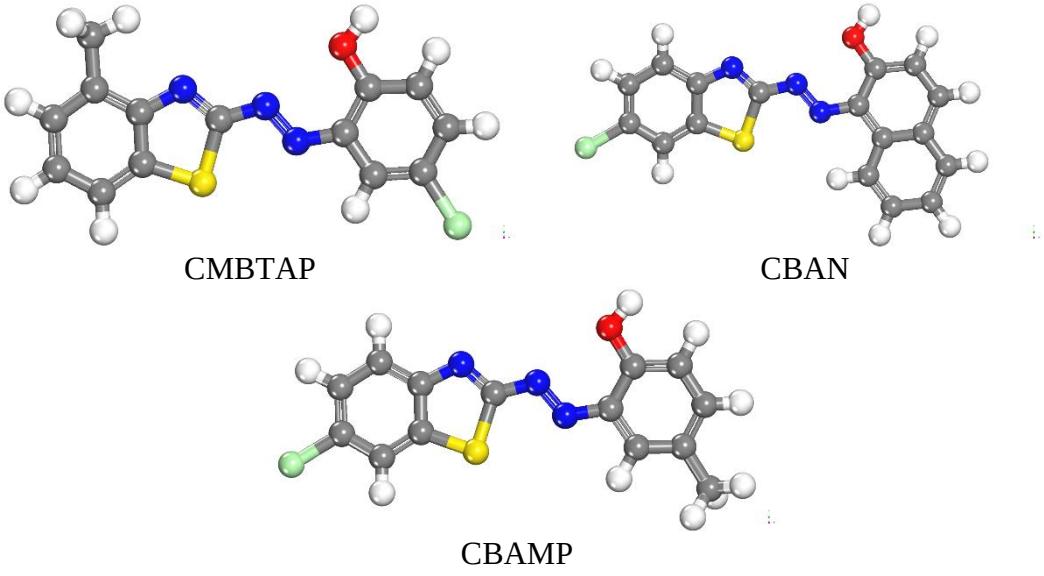


Figure S10. The optimized molecular structures of the investigated benzothiazole dyes.

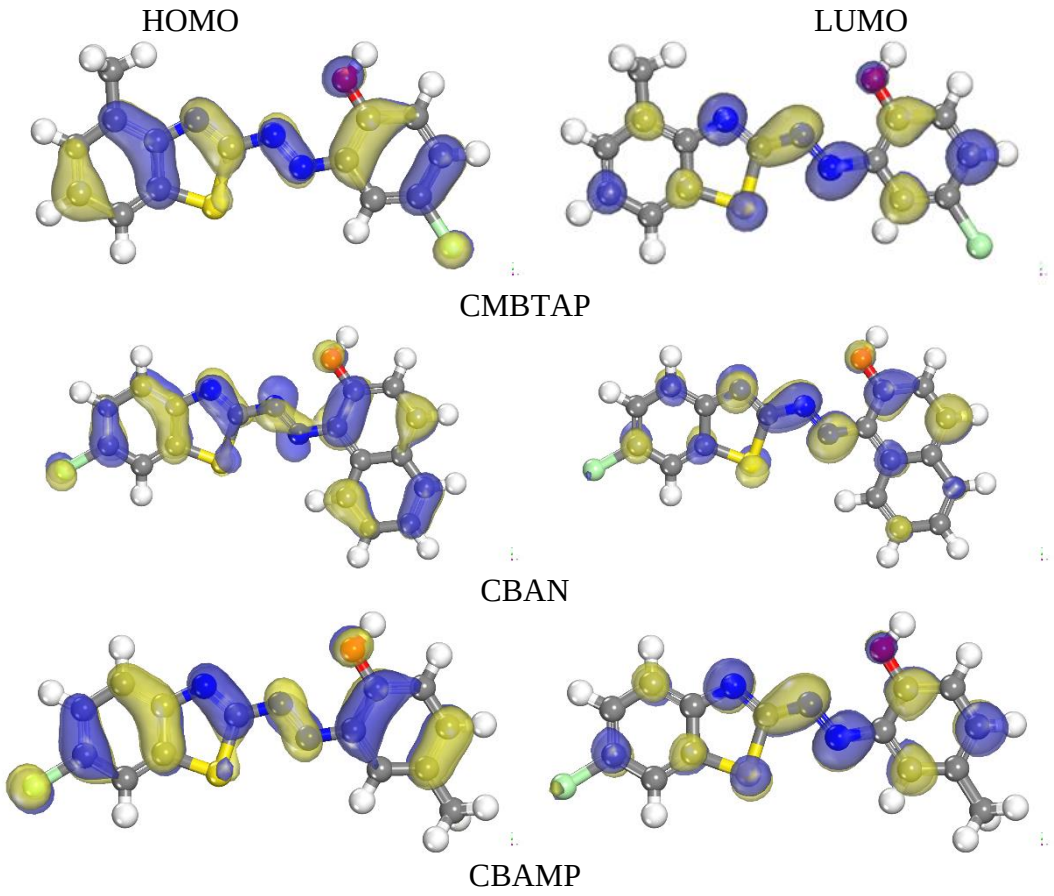
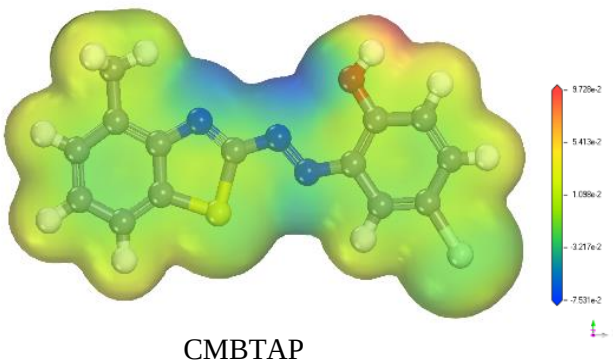
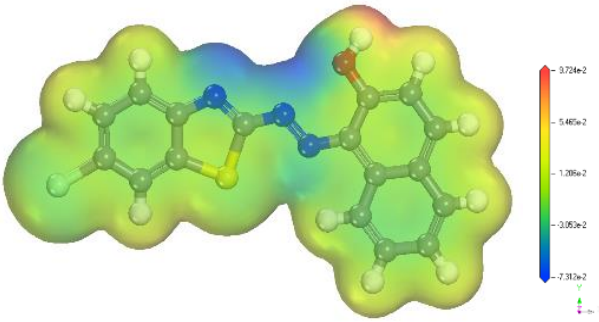


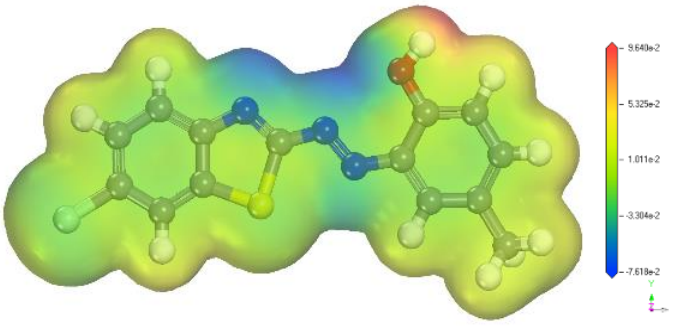
Figure S11. The highest occupied molecular orbital and the lowest unoccupied molecular orbital of the investigated benzothiazole dyes.



CMBTAP



CBAN



CBAMP

Figure S12. The molecular electrostatic potentials of optimized structures of the investigated benzothiazole dyes.

Table S1. Synergism Parameter (S_Θ) at Different Concentrations of Inhibitors

Inhibitor	Synergism parameter (S_Θ)		
	Conc. x 10^{-5} M	**Impedance**	**Polarization**
CMBTAP	1	2.57	2.62
	5	2.56	3.04
	10	2.57	3.01
	15	2.61	2.85
	20	3.23	3.66
CBAN	1	1.86	1.83
	5	2.10	1.75
	10	2.17	2.26
	15	2.16	2.04
	20	2.13	1.91
CBAMP	1	2.33	2.51
	5	2.53	2.75
	10	2.61	2.87
	15	2.78	2.86
	20	2.77	2.92

Table S2. Outputs and Descriptors Calculated by the Monte Carlo Simulation for Adsorption of the Inhibitors on Fe (110) Surface

Compound	Total energy (Kcal/mol)	Adsorption energy (Kcal/mol)	Rigid adsorption energy (Kcal/mol)	Deformation energy (Kcal/mol)	Dye: dEad/dNi	HCl: dEad/dNi	H_2O : dEad/dNi	H_3O: dEad/dNi	I^-: dEad/dNi
I^-	-5635.13	-13517.17	-5932.79	-7584.38	---	-8.02	-33.14	-169.42	-136.96
CMBTAP	-5634.88	-13549.25	-5939.32	-7609.94	-212.72	-7.27	-33.80	-171.42	---
CMBTAP+ I^-	-5722.39	-13636.76	-6024.99	-7611.77	-222.74	-5.79	-32.93	-165.21	-131.47
CBAN	-5441.95	-13469.77	-5858.18	-7611.59	-90.20	-8.02	-32.59	-167.65	---
CBAN+ I^-	-5558.84	-13566.66	-5961.02	-7605.65	-142.25	-7.87	-32.60	-167.47	-131.46
CBAMP	-5580.61	-13482.65	-5876.28	-7606.38	-113.76	-7.14	-32.85	-166.86	---
CBAMP+ I^-	-5669.22	-13571.26	-5962.74	-7608.53	-160.30	-8.82	-33.09	-163.53	-131.57