Supplementary information

Inhibitory behaviour and adsorption stability of benzothiazole derivatives as corrosion inhibitor towards galvanised steel

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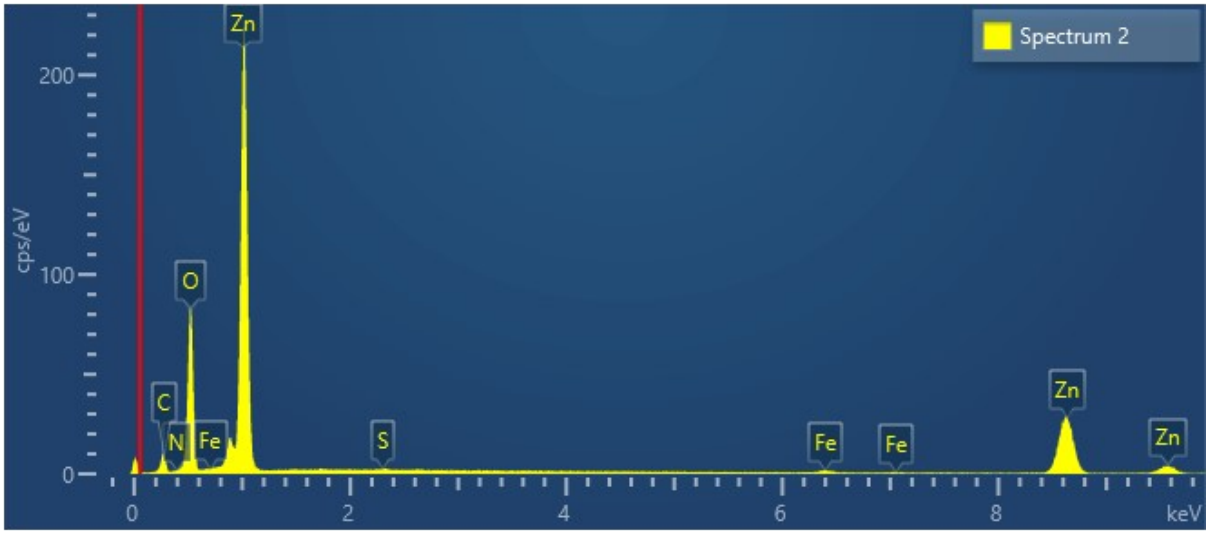

Figure S1. Chemical composition of ZE surface after 90-min immersion in 0.1 M NaCl solution with 1 mM 2-ABT.

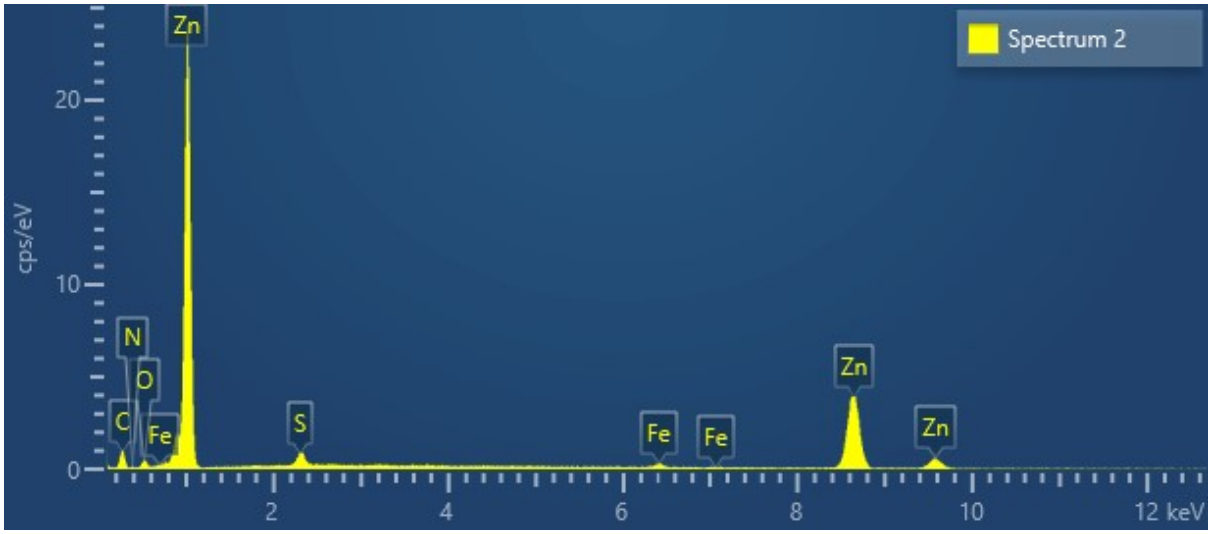

Figure S2. Chemical composition of ZE surface after 90-min immersion in 0.1 M NaCl solution with 1 mM 2-MBT.

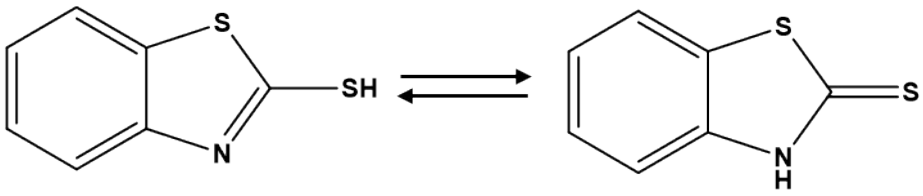

Figure S3. Tautomeric form of 2-MBT. Thiol form (left); thione form (right).

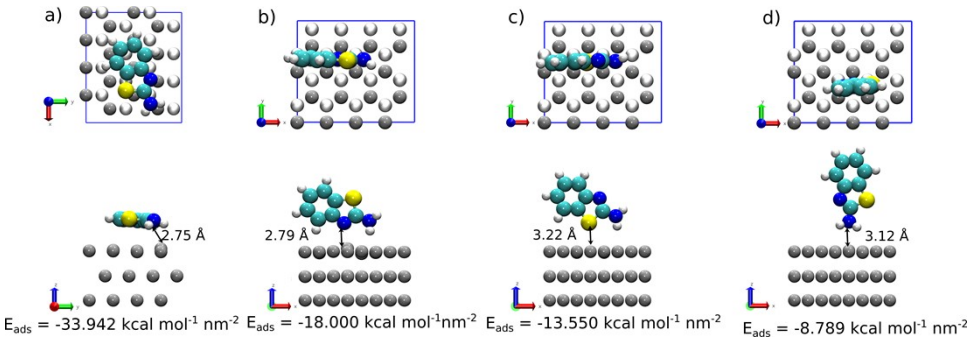

Figure S4. Top view and side view for the final adsorption structures at low concentration (1 molecule/nm^2 obtained for 2-ABT on Zn {0001}: a) Parallel, b) (N, NH_2)-Zn, c) (S, NH_2)-Zn, and d) (NH_2)-Zn. White, cyan, yellow, blue, and gray colored spheres represent H, C, S, N, and Zn atoms. On the top view of each case, degraded color spheres represent the Zn under the surface. The adsorption energy (Eads) for each case is shown below the view side of the structure.

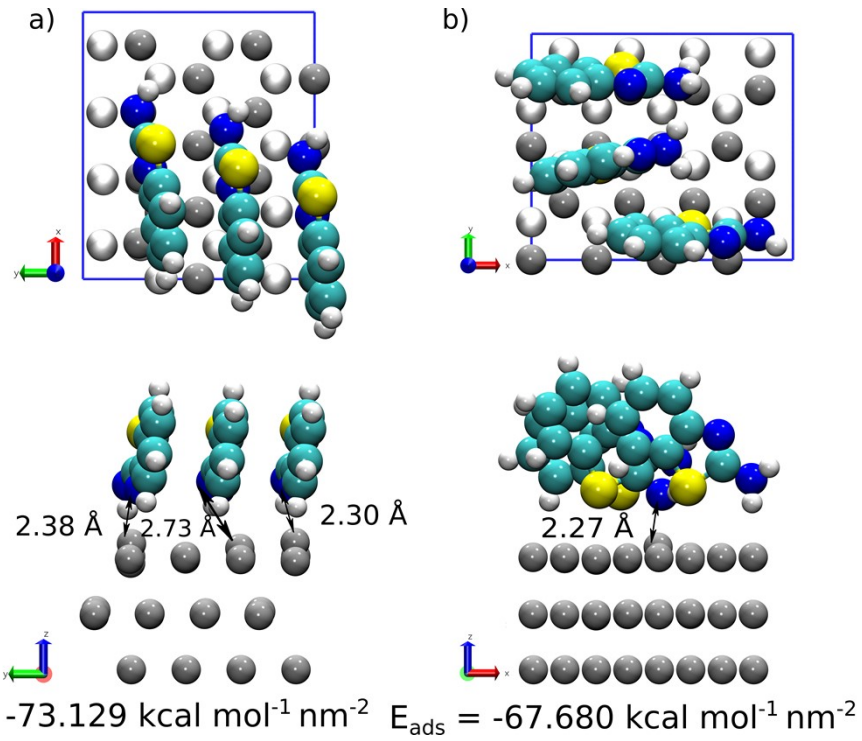

Figure S5. Top view and side view for the final adsorption structures at high concentration (3 molecule/nm^2 obtained for 2-ABT on Zn {0001}: a) (N, NH_2)-Zn, and b) (S, NH_2)-Zn cases. White, cyan, yellow, blue, and gray colored spheres represent H, C, S, N, and Zn atoms. On the top view of each case, degraded color spheres represent the Zn under the surface. The adsorption energy (E_{ads}) for each case is shown below the view side of the structure.

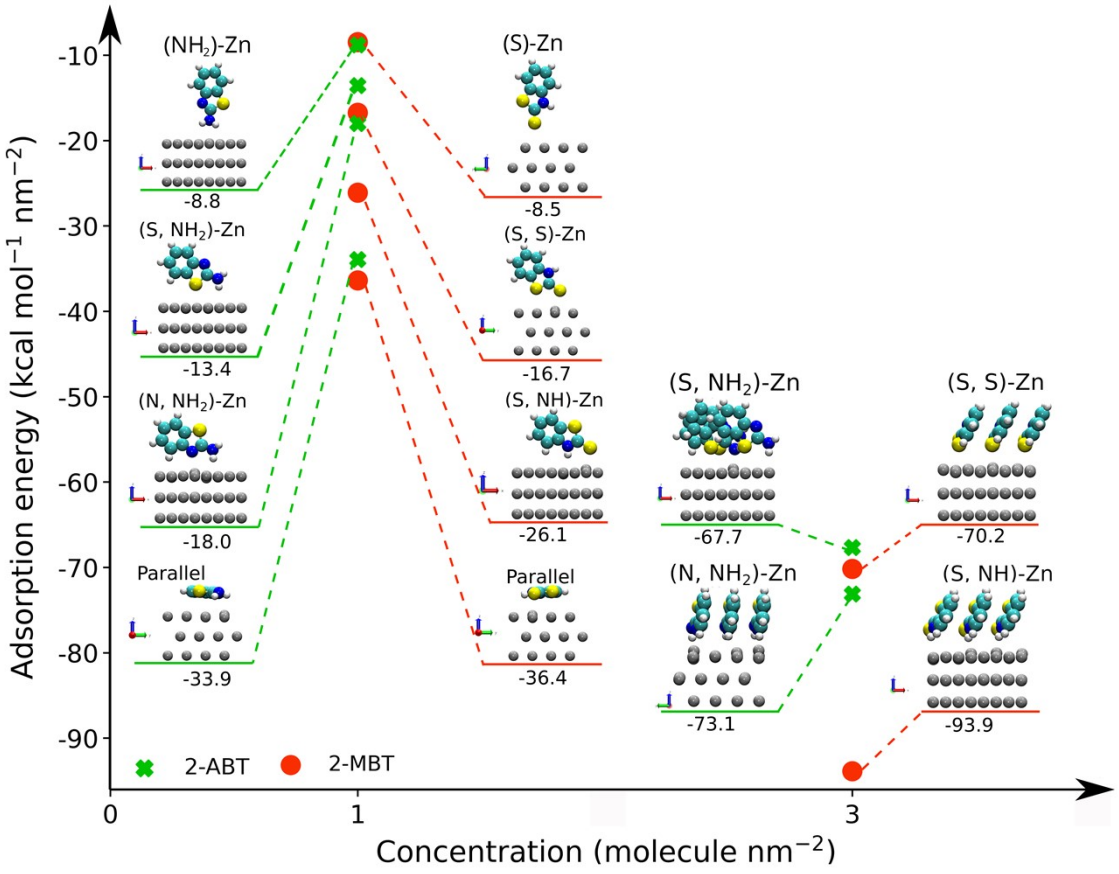

Figure S6. Different adsorption configurations for 2-ABT and 2-MBT at low (one $molecule\ /\ cell$) and high (three $molecules\ /\ cell$) concentration on the Zn{0001} surface. White, cyan, yellow, blue, and gray colored spheres represent H, C, S, N, and Zn atoms. The orange and green points represent the adsorption energy (E_{ads}) per surface area [$kcal\ mol^{-1}\ nm^{-2}$], which appears below the side view of each structure.

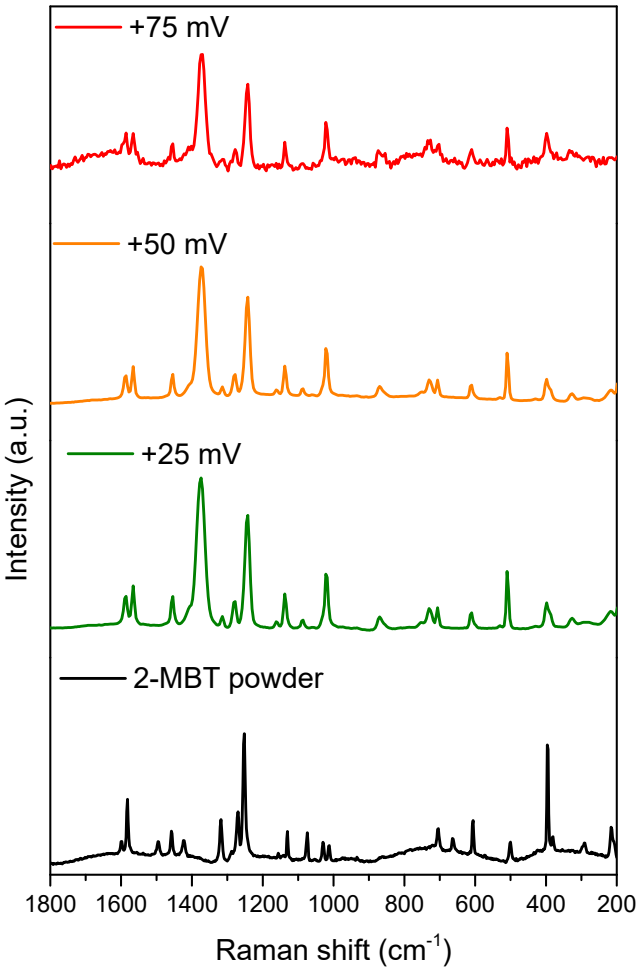

Figure S7. Raman spectra of 2-MBT powder and ZE inhibited surface after 2-h polarisation (0 - +75 mV) in the inhibited solution of 1 mM 2-MBT.

Table S1. Adsorption energies without normalize by surface area [kcal mol^{-1}], and adsorption energies per molecule [kcal mol^{-1}/molecule] for the 2-ABT and 2-MBT SAM cases.

	Adsorption mode	Adsorption energy [kcal mol^{-1}]	Adsorption energy per molecule [kcal mol^{-1}/molecule]
2-ABT	(N, NH2)-Zn	-73.870	-6.440
	(S, NH2)-Zn	-68.366	-9.102
2-MBT	(S,NH)-Zn	-94.835	-5.232
	(S, S)-Zn	-70.895	-6.724