Supporting Information

Multidimensional Insights Involving Electrochemical and in Silico Investigation into the Corrosion Inhibition of Newly Synthesized Pyrazolotriazole Derivatives on Carbon Steel in HCl Solution

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1. ^{1}H NMR and ^{13}C spectra of CPT and MPT

The NMR spectra were measured on a Bruker Avance DPX300 instrument. The chemical shifts (δ) are expressed in ppm down field from TMS taken as an internal reference. The samples are ionized by the ion spray technique (IS). TLC and column chromatography were carried out respectively on silica plates (Merck 60 F254) and silica gel (Merck 60, 230-400 mesh). The ^{1}H NMR and ^{13}C spectra of CPT and MPT are shown in Fig. S1~S4.

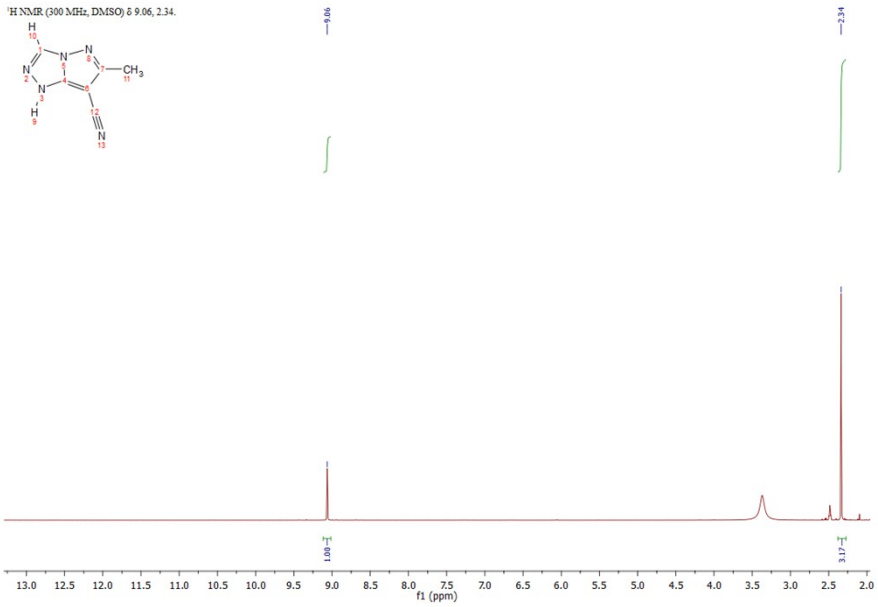

Fig. S1. The ^{1}H-NMR of CPT.

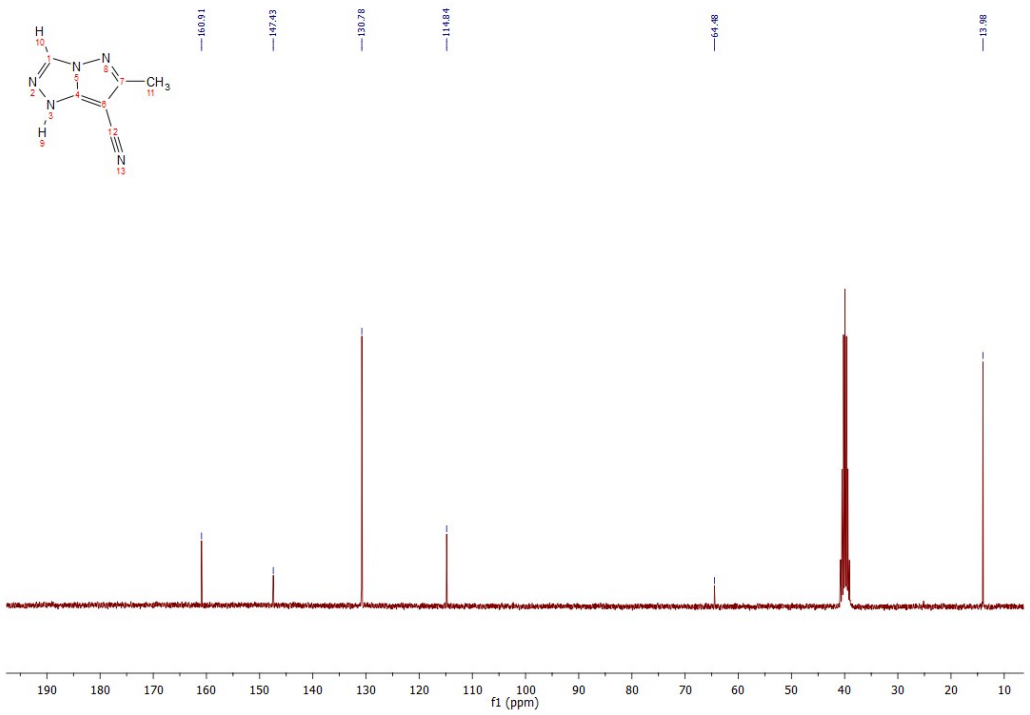

Fig. S2. The ^{13}C-NMR of CPT.

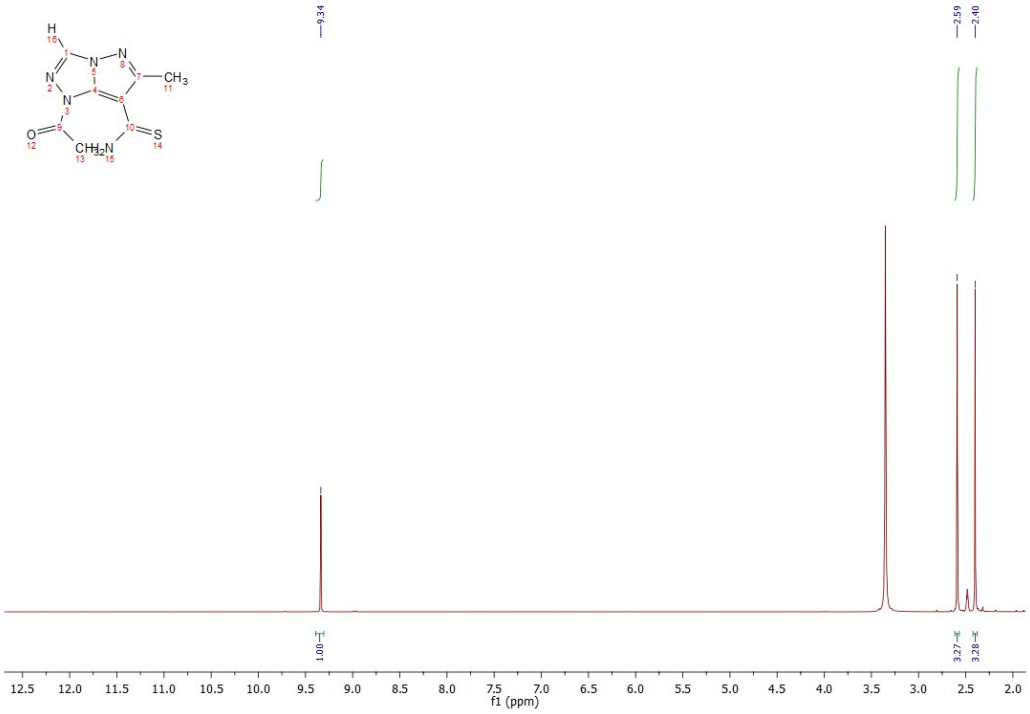

Fig. S3 The ^{1}H-NMR of MPT.

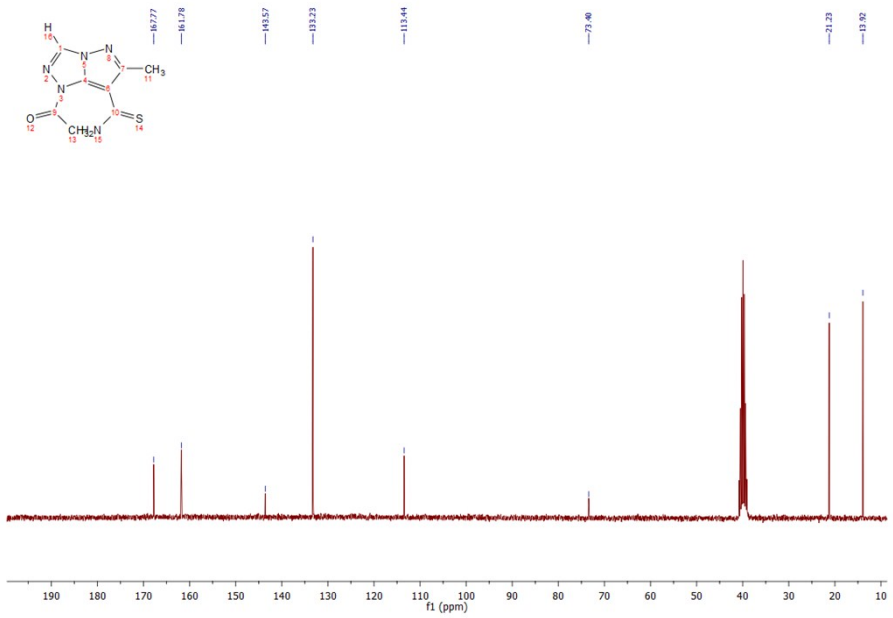

Fig. S4 The ^{13}C-NMR of MPT.

2. Toxicity evaluation

The TOPKAT module of Discovery studio 3.0 software was employed to evaluate the toxicity of CPT amd MPT. Several important toxicity endpoints involving carcinogenicity (C), mutagenicity (M), biodegradability (B), and skin irritation (SI) were chosen to represent the toxicities. All calculations were based on the method of QSARs, which are mathematical models that are used to predict toxicity from physical characteristics of the molecular structure. Table S1 shows the computed probability data for CPT and MPT inhibitors. According to TOPKAT calculation theory, every toxicity endpoint corresponds to a probability value which specifically represents the toxicity degree of inhibitors.[1] Probability values from 0.00 to 0.30 represent low toxicity probabilities while probability values >0.70 indicate high toxicity probabilities. The value of probabilities >0.30 but <0.70 is considered as indeterminate.[2] According to the data in Table S1, the obtained probability values indicate that the toxic levels of both inhibitors are in the safe area.

Table S1 The computed probability data for CPT and MPT inhibitors.

Inhibitor	Carcinogenicity (C)	Mutagenicity (M)	Biodegradability (B)	Skin Irritation (SI)
CPT	0.004	0.363	0.153	0.003
MPT	0.006	0.000	0.000	0.000

3. Molecular dynamics simulation

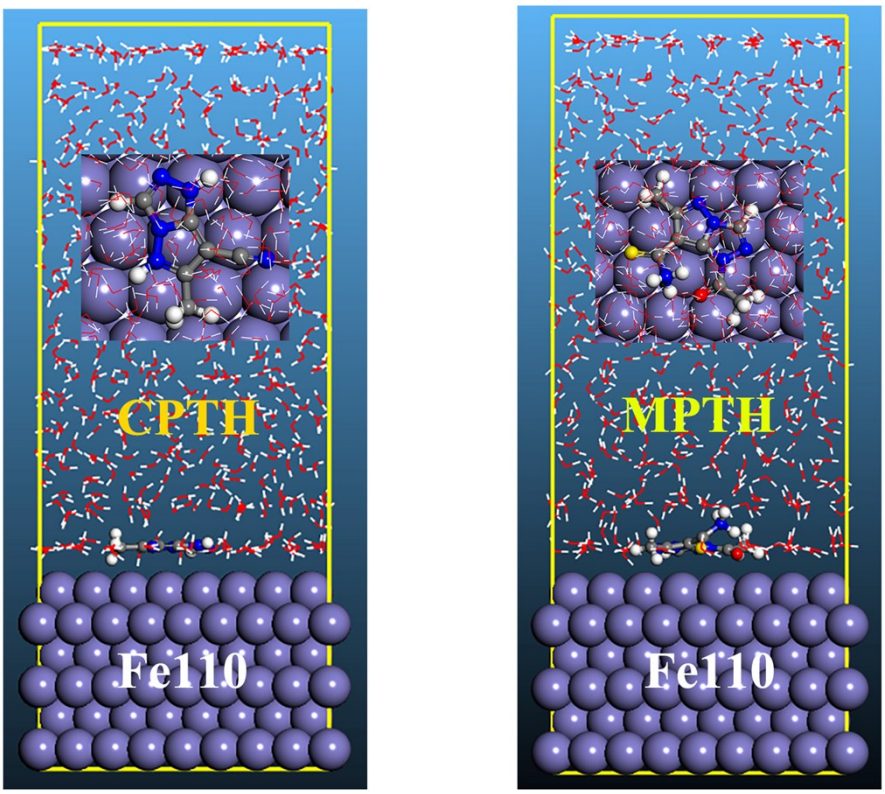

Fig. S5 Equilibrium configurations for CPTH and MPTH inhibitors on Fe(110) surface.

References

1. R. D. Snyder, G. S. Pearl, G. Mandakas, W. N. Choy, F. Goodsaid and I. Y. Rosenblum, *Environ. Mol. Mutagen.*, 2004, **43**, 143-158.
2. R. Srikala and M. N. Babu, *Int. J. Pharm. Sci. Res.*, 2018, **9**, 286-291.