

Supporting Information

The Anti-corrosive Behavior of Benzo-Fused N-Heterocycles: An In-Silico Study Toward Developing Organic Corrosion Inhibitors

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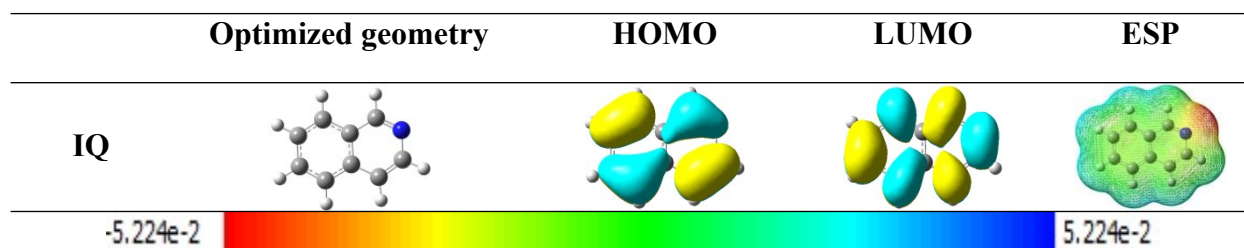
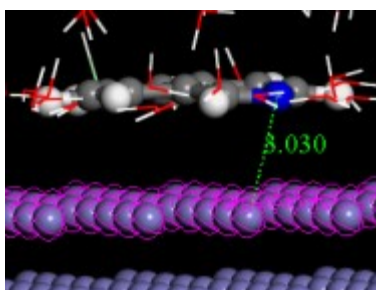
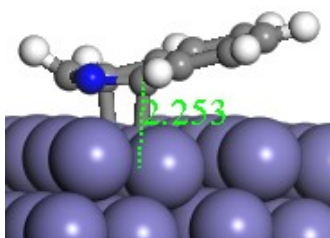


Fig. S1. Optimized geometry, FMOs density distributions, and electrostatic potential (ESP) structures of IQ molecule using DFT/6-311++G (d, p) level of theory.



IQ

Fig. S2. The most stable configurations for adsorption of the IQ molecule on Fe(110) surface using MC simulations.



IQ

Fig. S3. The most stable adsorption configurations for the IQ/Fe(110) systems. The length of chemical bonds is shown in the graph.

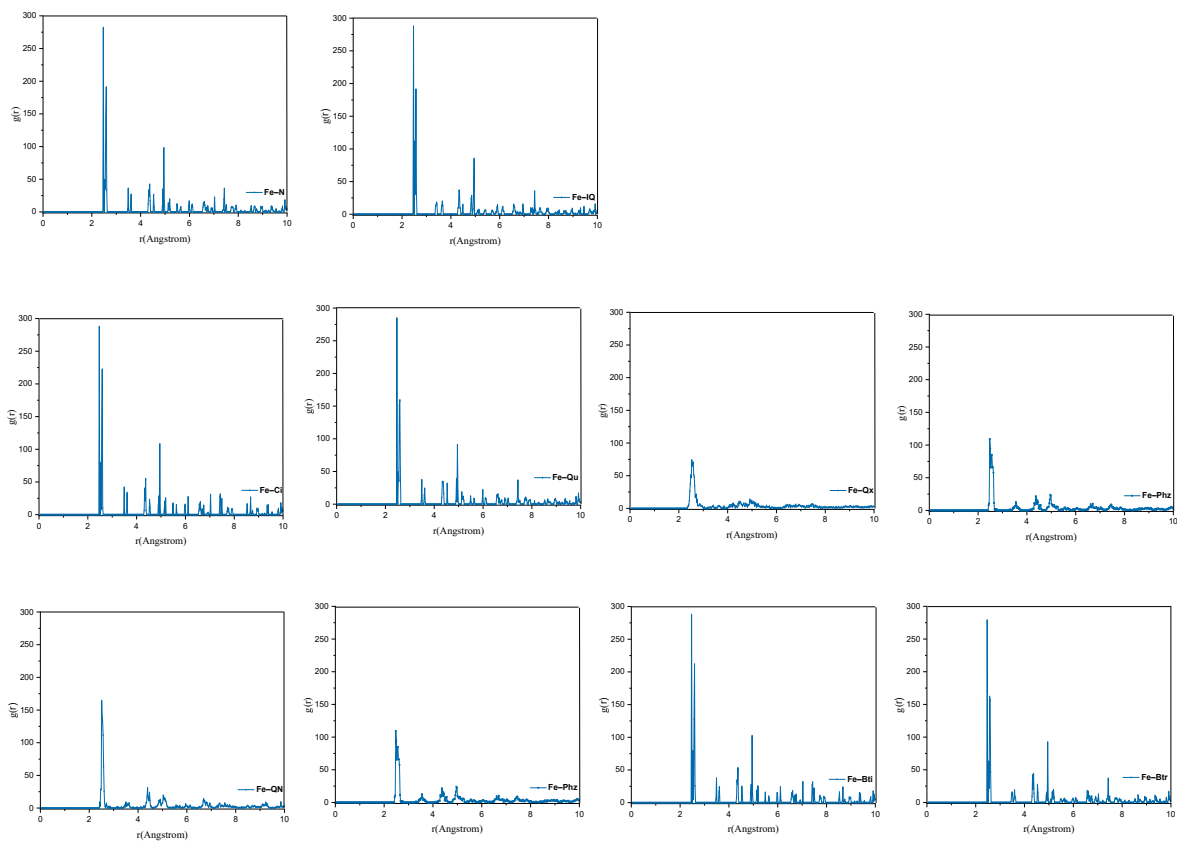
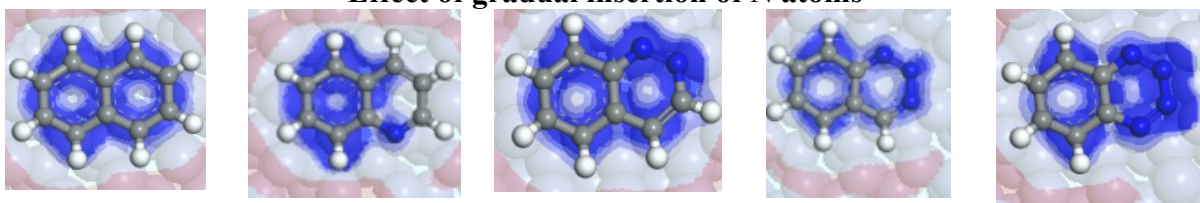


Fig. S4. RDF curves of studied inhibitors interacting with Fe (1 1 0) plane obtained after MD simulation.

Effect of gradual insertion of N atoms



N

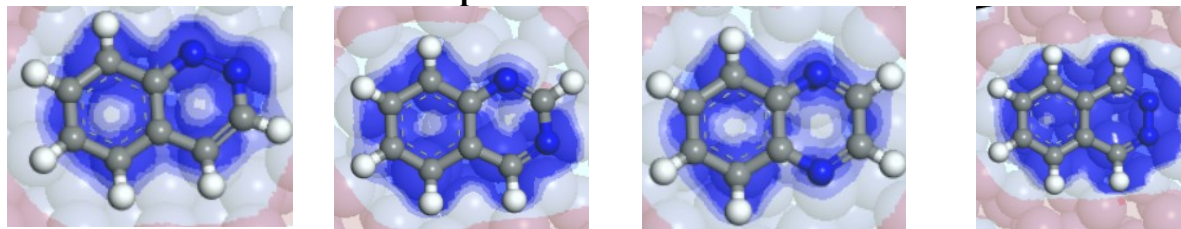
QN

Ci

Bti

Btr

Effect of positional isomerism of N atoms



Ci

Qu

Qx

Phz

Fig. S5. Charge density difference for the studied adsorption systems. The red region indicates the loss of electrons, while electron accumulation is indicated in blue. (Cutoff value of $\pm 0.002 e \text{ \AA}^{-3}$).

Table S1: Theoretical ionization potential energies of inhibitors and their available experimental ionization potential energies

Molecule		
N	8.16 [1]	8.17
QN	8.67 [2]	8.69
IQ	8.55 [3]	8.60
Ci	8.95 [3]	9.11
QX	9.01 [4]	9.10
Phz	9.22 [3]	9.32

Table S2: Natural atomic charges of studied inhibitors using DFT/6-311++G (d, p) level of theory

Atom	X ₁	X ₂	X ₃	X ₄	C _{4a}	C ₅	C ₆	C ₇	C ₈	C _{8a}
Effect of gradual insertion of N atoms										
N	-0.18	-0.20	-0.21	-0.16	-0.07	-0.18	-0.20	-0.20	-0.18	-0.05
IQ	0.10	-0.45	0.03	-0.22	-0.04	-0.18	-0.18	-0.20	-0.16	-0.10
QN	-0.44	0.07	-0.25	-0.14	-0.09	-0.18	-0.20	-0.19	-0.18	0.17
Bti	-0.21	-0.01	-0.27	0.09	-0.11	-0.17	-0.18	-0.18	-0.17	0.14
Btr	-0.18	-0.04	-0.04	-0.18	0.11	-0.18	-0.17	-0.17	-0.18	0.11
Effect of positional isomerism of N atoms										
Ci	-0.20	-0.22	-0.01	-0.18	-0.07	-0.19	-0.18	-0.20	-0.17	0.13
Qu	-0.46	0.28	-0.48	0.13	-0.14	-0.17	-0.20	-0.18	-0.19	0.18
Qx	-0.40	0.03	0.03	-0.40	0.13	-0.18	-0.19	-0.19	-0.18	0.13
Phz	0.07	-0.25	-0.25	0.07	-0.08	-0.17	-0.15	-0.15	-0.17	-0.08

Table S3: The computed adsorption parameters by Monte Carlo simulation (in kcal/mol)

	Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	dE_{ad}/dN_i		
					Inh.	H ₂ O	HCl
IQ	-2611.84	-2715.12	-2858.17	143.05	-95.95	-14.68	-5.81

Table S4: Bond length (BL, Å) between the **IQ** atoms and the iron surface atoms as well as their type of interactions (T, Top; H, Hallow; B, Bridge)

IQ	
BL	Type

X₁	2.25	T
X₂	2.59	H
X₃	2.27	H
X₄	2.26	B
C_{4a}	2.90	H
C₅	2.73	T
C₆	3.20	H
C₇	2.93	H
C₈	2.72	T
C_{8a}	2.89	H

References

1. R. A.W. Johnstone, F. A. Mellon, S. D.Ward, Online acquisition of ionization efficiency data, Intern. J. Mass Spectrom. Ion Phys., 5 (1970) 241.
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3. A. J. Yench, M. A. El-Sayed, Lowest ionization potentials of some nitrogen heterocyclics, J. Chem. Phys. 48 (1968) 3469.
4. F. Brogli, E. Heilbronner, T. Kobayashi, Photoelectron spectra of azabenzenes and azanaphthalenes: II. A reinvestigation of azanaphthalenes by high-resolution photoelectron spectroscopy, Helv. Chim. Acta 55 (1972) 274.