:Supplementary File:

Molecular dynamics and density functional theory study on corrosion inhibitory action of three substituted pyrazine derivatives on steel surface

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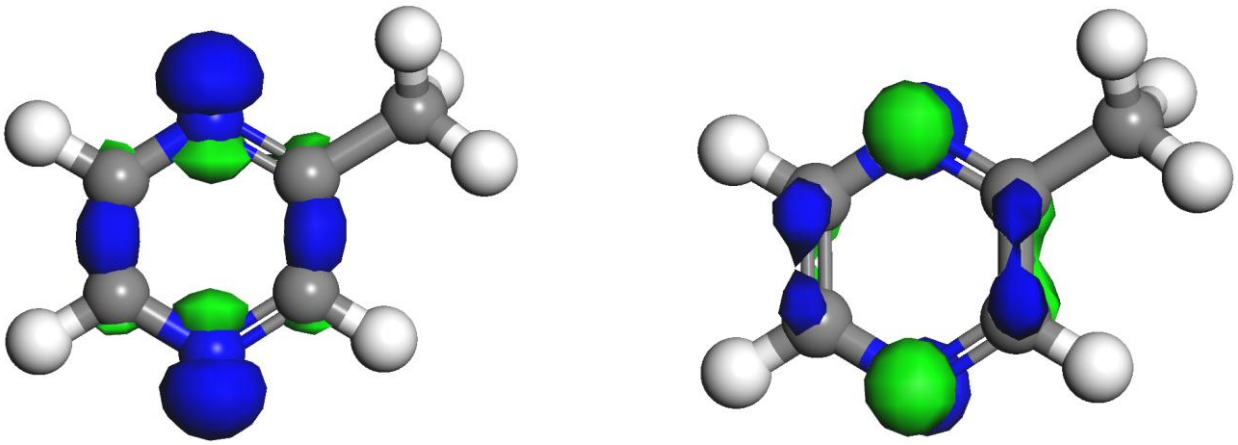
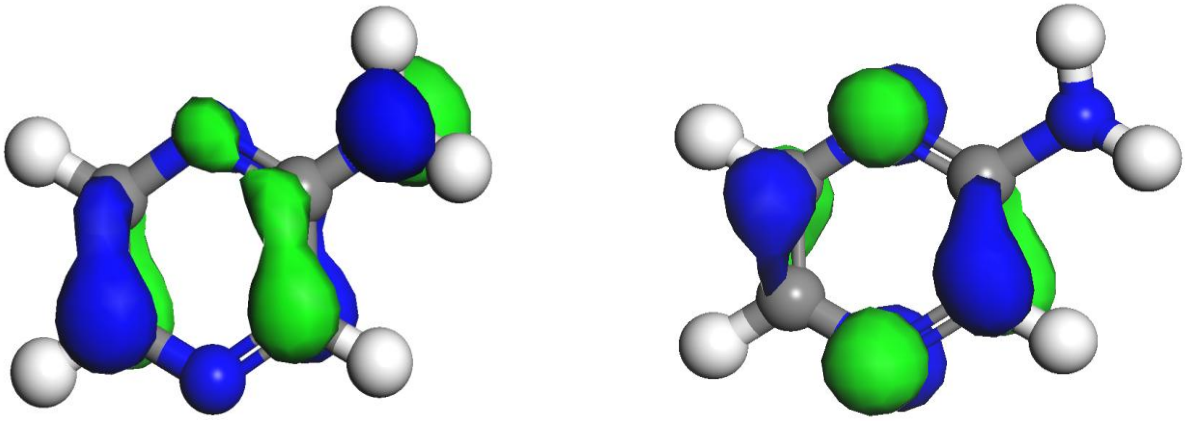


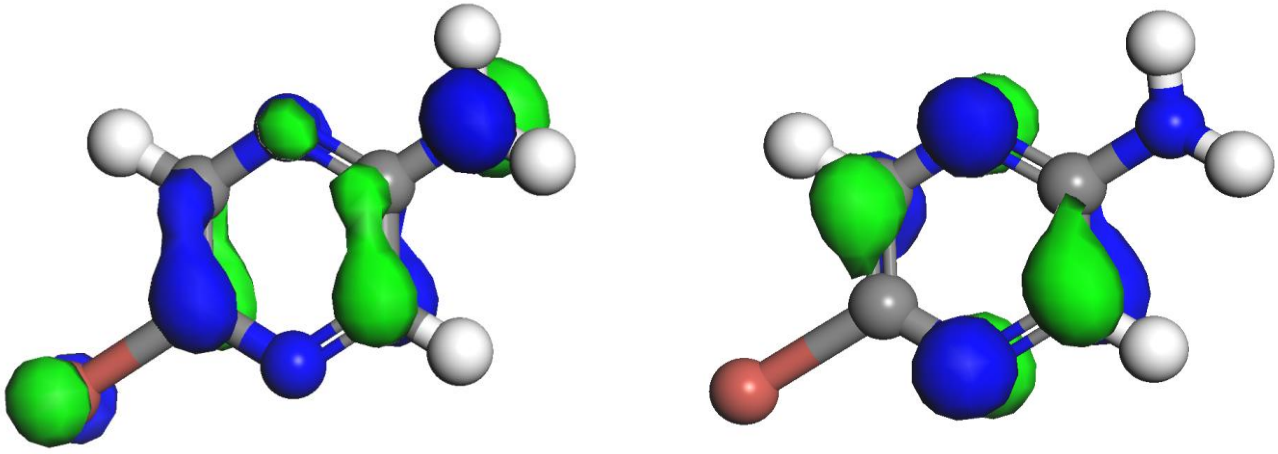
(a) (b)

Figure S1. DFT derived (Dmol^3) Frontier molecular orbital density distribution: (a) HOMO and (b) LUMO plot of MP ligand.



(a) (b)

Figure S2. DFT derived (Dmol^3) Frontier molecular orbital density distribution: (a) HOMO and (b) LUMO plot of AP ligand.



(a) (b)

Figure S3. DFT derived (Dmol^3) Frontier molecular orbital density distribution: (a) HOMO and (b) LUMO plot of ABP ligand.

Table S1. Calculated quantum chemical parameters of the studied inhibitors.

Inhibitor	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	$I = -E_{HOMO}$	$A = -E_{LUMO}$	χ	η	ΔN
MP	-6.986	-1.549	5.437	6.986	1.549	4.2675	2.7185	0.502
AP	-6.275	-1.326	4.949	6.275	1.326	3.8005	2.4745	0.646
ABP	-6.414	-1.817	4.597	6.414	1.817	4.1155	2.2985	0.627