

Table S1. Inhibition was statistically compared to the efficacy of other heterocyclic organic Inhibitors that had previously been investigated

Corrosion Inhibitor	Metal	Corrosive solution	% efficiency	Ref.
(E)-N0 -(2,4-dimethoxybenzylidene)-2-(6-methoxynaphthalen-2-yl)propanehydrazide	MS	1 M HCl	95.7-95	1
N0-cyclohexylidene-2-(6-methoxynaphthalen-2-yl) propanehydrazide	MS	1 M HCl	86.0	1
Furoin thiosemicarbazone	MS	1 M HCl	89.7	2
4-pyridinecarboxaldehyde thiosemicarbazone	MS	1 M HCl	85.5	3
5-hexylsulfanyl-1,2,4-triazole	MS	1 M HCl	97.0	4
3-(3-formyl-4-hydroxy- 1-phenylazo) - 1, 2, 4-triazole	Cu	1 M HNO ₃	95.8	5
3-(3-formyl-4-hydroxy- 1-phenylazo) - 1, 2, 4-triazole	MS	1M HCl	92.8	6
2- , 2-amino-7-hydroxy-4-(4-methoxyphenyl)-1,4 dihydroquinoline-3 carbonitrile	MS	1 M HCl	96.6	6
2- , 2-amino-7-hydroxy-4-(4-methoxyphenyl)-1,4 dihydroquinoline-3 carbonitrile	MS	1 M HCl	98.0	6
2-amino-7-hydroxy-4-phenyl-1,4-dihydroquinoline-3-carbonitrile	MS	HCl	93.3	6
2-amino-7-hydroxy-4-(p-tolyl)-1,4 dihydroquinoline-3-carbonitrile	MS	HCl	92.8	6
5-(2- Hydroxyphenyl)-2,7-dithioxo-2,3,5,6,7,8-hexahydropyrimido [4,5-d]-pyrimidin-4(1H) one	N80 steel	1 M HCl	73.1	7
5-(2,5-dimethylthiophen-3yl)-4-(4-(6-(2,5-dimethylthiophen-3-yl)-2- hydroxypyrimidin-4-yl)phenyl)pyrimidin-2-ol	MS	H ₂ SO ₄	98.3	8
5-(2,5-dimethylthiophen-3yl)-4-(4-(6-(2,5-dimethylthiophen-3-yl)-2-mercaptopyrimidin-4-yl)phenyl) pyrimidin-2-thiol	MS	H ₂ SO ₄	99.3	8
5-(2,5-dimethylthiophen-3yl)-4-(4-(6-(2,5-dimethylthiophen-3-yl)-2-mercaptopyrimidin-4-yl)phenyl) pyrimidin-2-thiol	MS	H ₂ SO ₄	99.3	8
2-((6-methyl-2-ketoquinoUne-3-yl)methylene) hydrazinecarbothioamide	MS	1 M HCl	95.8	9
5,50-(1,4-phenylene)bis(N-phenyl-1,3,4-thiadiazol-2-amine)	MS	1 M HCl	94.0	10
(Z)-2-tert-butylimino-3-isopropyl-5-phenyl-1,3,5-thiadiazinane-4-one (Buprofezin)	CS	1 M HCl	91.3	Our results

References

1. Chaouiki, A.; Chafiq, M.; Lgaz, H.; Al-Hadeethi, M.; Ali, I.; Masroor, S.; Chung, I. Green Corrosion Inhibition of Mild Steel by Hydrazone Derivatives in 1.0 M HCl. *Coatings* **2020**, *10*, 640.
2. Jacob, K.; Parameswaran, G. Corrosion inhibition of mild steel in hydrochloric acid solution by Schiff base furoin thiosemicarbazone. *Corros. Sci.* **2010**, *52*, 224–228.

3. Xu, B.; Yang, W.; Liu, Y.; Yin, X.; Gong, W.; Chen, Y. Experimental and theoretical evaluation of two pyridine carboxaldehyde thiosemicarbazone compounds as corrosion inhibitors for mild steel in hydrochloric acid solution. *Corros. Sci.* **2014**, *78*, 260–268.
4. Naciri, M.; El Aoufir, Y.; Lgaz, H.; Lazrak, F.; Ghanimi, A.; Guenbour, A.; Ali, I.; El Moudane, M.; Taoufik, J.; Chung, J. Exploring the potential of a new 1,2,4-triazole derivative for corrosion protection of carbon steel in HCl: A computational and experimental evaluation. *Colloids Surf. A Physicochem. Eng. Asp.* **2020**, *597*, 124604.
5. Madkour, L.; Kaya, S.; Obot, I. Computational, Monte Carlo simulation and experimental studies of some arylazotriazoles (AATR) and their copper complexes in corrosion inhibition process. *J. Mol. Liq.* **2018**, *260*, 351–374.
6. Singh, P.; Srivastava, V.; Quraishi, M. Novel quinoline derivatives as green corrosion inhibitors for mild steel in acidic medium: Electrochemical, SEM, AFM, and XPS studies. *J. Mol. Liq.* **2016**, *216*, 164–173.
7. Haque, J.; Ansari, K.R.; Srivastava, V.; Quraishi, M.A.; Obot, I.B. Pyrimidine derivatives as novel acidizing corrosion inhibitors for N80 steel useful for petroleum industry: A combined experimental and theoretical approach. *J. Ind. Eng. Chem.* **2017**, *49*, 176–188.
8. Amusia, N.; Saranya, J.; Sounthari, P.; Zarrouk, A.; Chitr, S. Corrosion inhibition and adsorption behavior of some bipyridine derivatives on mild steel in acidic medium. *J. Mol. Liq.* **2017**, *225*, 406–417.
9. Al-Baghdadi, S.B.; Al-Amiery, A.A.; Gaaz, T.S.; Kadhum, A.A.H. Terephthalohydrazide and isophthalo-hydrazide as new corrosion inhibitors for mild steel in hydrochloric acid: Experimental and theoretical approaches. *Koroze Ochr. Mater.* **2021**, *65*, 12–22.
10. Al-Amiery, A.A. Anti-corrosion performance of 2-isonicotinoyl-n-phenylhydrazine carbothioamide for mild steel hydrochloric acid solution: Insights from experimental measurements and quantum chemical calculations. *Surf. Rev. Lett.* **2021**, *28*, 2050058.