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Assessing the Environmental Safety of Corrosion Inhibitors in Iraqi Studies: A Predictive Analysis

Kafa Khalaf Hammud*

Iraqi Atomic Energy Commission, Iraq

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Corresponding Author:
Kafa Khalaf Hammud
kafaakhalaf@gmail.com

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Abstract

Corrosion inhibitors play a crucial role in mitigating the detrimental effects of chemical and electrochemical interactions over time. This phenomenon poses significant threats to structural integrity, strength, and has far-reaching economic implications across various industries such as construction, petrochemicals, mining, fertilizer, and energy units. The environmental repercussions, including toxic outflows and plant failures, underscore the need for comprehensive assessments. Despite the commendable contributions of Iraqi researchers in developing organic, inorganic, natural, and nano-corrosion inhibitors, there is a critical gap in considering potential side effects. This study explores a pioneering approach to evaluating the toxicity of corrosion inhibitors on both human health and the environment. Leveraging mathematical modeling and mechanisms, we present a mimic estimation of environmental factors influencing corrosion phenomena. The out-lab experimental calculations employ Quantitative Structure-Activity Relationship (QSAR) techniques, providing a structural-based predictive model for assessing the potential impact of chemicals before embarking on experimental complexities. Drawing from Iraqi journals, seven corrosion inhibitors with diverse chemical structures, experimental conditions, and publishing sources were selected. These compounds were subjected to scrutiny using online prediction websites that evaluate Embro-toxicity, Cardio-toxicity, and crop-toxicity. Each inhibitor underwent screening by specific toxicological web servers. The findings revealed that all studied compounds posed moderate to extremely unsafe risks to fetal health during pregnancy, potentially categorizing them as teratogens with elevated risks of preterm labor, miscarriage, or stillbirth. Additionally, none of the tested materials exhibited herbicidal activity.

1. Introduction

1.1. General Preface

Corrosion is the consequence of chemical and electrochemical interactions over time in metallics and non-metallics because of their environment where metal has great energy had to be release and form stable state(s). For example, corrosion of iron or its alloys considers as damages in structure and loss strength leading to

economic and industrial fears need a sustainable research looking for solutions. Corrosion is the source structural damage in many life fields like construction, petrochemicals, mining, fertilizer, energy units, and other industrial components leading to toxic chemical outflows and plant failure [1]. Corrosion electrochemical reactions are hydrogen evolution and oxygen reduction and occurred according to composition, atomic structure, scopic limitations in both macro- and micro- range, and mechanical response such as tensile or compressive, chemical nature of the environment, temperature, and other factors. Various review articles and books associated to this title have been published based on classification, application, classification, and mechanism as well as recent trends of organic molecules with hetero atoms and π-electron atom or group, inorganic salts and eco-friendly phyto-constituents [2, 3].

1.2. Iraqi Academic Research: Advancements in Corrosion Inhibitors

According to Iraqi Academic Scientific Journal website, Iraqi researchers had excellent contributions in corrosion subject especially corrosion inhibitors. They intensively investigated organic, inorganic, natural, and nano-materials. For example, Al- Saadie et al. in 2007 studied corrosion behavior of zinc in acidic medium (1 M HCl) using urea with low concentration range (0.001 – 0.005) M at (285-328) K by weight loss measurement where highest protection efficiency was 88% with 0.005M [4]. Also, Benzotrizole was reacted as a mixed copper corrosion inhibitor in oxygenated 0.1M H_2SO_4 and evaluated by potentiostatic polarization at (283,288,293, and 298) K where 0.01M was effective inhibitor with efficiency was 98% with formation of Cu-BTA film [5].

In another study, pure aluminum in aqueous 3.5% sodium chloride solution was subjected to corrosion inhibition study with ampicillin. Potentiodynamic polarization confirmed that ampicillin lowered corrosive effect of saline solution spontaneously by forming monolayer on the surface according to Langmuir adsorption isotherm and quantum mechanical -B3LYP/6-31G basis set [6].

Reheem published a study about mixed materials: sodium phosphate as corrosion inhibitor and sodium glocunate as a scale dispersant. Weight loss method of carbon steel –cooling system saved from corrosion by these chemicals with efficiency reached 98%. She immersed carbon steel for (1-5) days with concentration range (20-80) ppm at temperatures of 25, 50, 75, and 100ºC [7].

In computational field, Oxazolidin-5- one (BIPNO5) was examined by Kubba and Al-Joborry as a corrosion inhibitor for carbon steel surface through Density Functional Theory (DFT) - B3LYP (6-311++G (2d, 2p) in vacuum, DMSO and water. Both found that this new hetero-derivative can be adsorb on carbon steel surface [8].
Engineering and Technology Journal in its pages (795-800) published another computational study of nano-dichlorobenzene molecules as corrosion inhibitors in oil pipeline sector by DFT at B3LYP level with (6-31G) basis sets. This article approved agreement between experimental and mathematical data. Here, nano-inhibitor minimized corrosion pipeline internal surfaces as the required goal [9].

Finding a new, nontoxic, cheap, and eco-friendly inhibitor for carbon steel in hydrochloric acid solution (1M, 2M, and 3M) was a good goal in Haleem study published in 2008 by Journal of Kerbala University. This important goal was done by hibiscus leaves with loss weight reached 77% (1M HCl) and 68% (3 M HCl) at 30 ºC through monolayer formation according to Langmuir adsorption isotherm [10].
Green corrosion inhibition continued by Iraqi researchers including Ajeel-2017 foundation of *Rosmarinus Officinalis* Leaves extract in 1M H_2SO_4 solution containing mild steel specimen. Weight loss and potentiostatic testing at room temperature presented 92% inhibition of 1000 ppm of this extract [11].

Milk thistle (*Silybum marianum*) is a natural plant in Iraq during spring period used for AA7051 aluminum alloy in NaOH solution in a range of temperatures by potentiodynamic polarization as a mixed–type inhibitor obeyed Langmuir isotherm [12]. Furthermore, aqueous extract of wild clary (20 mL/L) inhibited 83% of carbon steel corrosion of and a temperature of 298 (K) confirmed by Potentiostat, which revealed it as a mixed-type inhibition [13].

1.3. *In Silico* – Toxicity Prediction

All above mentioned studies and others that published in Iraqi journals searched how to minimize corrosion by chemical material. Corrosion inhibitors in these studies varied from natural extract, synthesized chemical, drug or other type of chemicals may be found in chemical labs. Excellent inhibition efficiency of any applied material seriously needs supported biological or medical studies to reduce toxicity in environment. To perform these investigations, time, cost, and hard trusted work stand as a strong wall for many academic works inside Iraq or other countries. To solve this problem, *in Silico* – toxicity prediction is a hope gate for many scientists.

Moreover, chemical(s) in short- or long-term experiments of *in vitro* as well as *in vivo* bio-metal or bio-nonmetal material mostly focused on preventing corrosion without taking in research account side effects. Mathematical modelling and mechanisms may mimic related environmental factors such as pH, temperature, concentration, chemical structure, etc. presenting in corrosion phenomena. Therefore, *in Silico* in **A**dsorption, **D**istribution, **M**etabolism, **E**xcretion, and **T**oxicity (**ADMET**) is out-lab experiment as mathematical calculations of **Q**uantitative **S**tructure - **A**ctivity **R**elationship (**QSAR**) [14]. Several research groups designed online computer simulation websites as free structural based prediction technique of chemical before accessing in complications of experiments and their results [15, 16, 17].

In this article, a new Iraqi attempt to present *in Silico* – online website prediction of seven chemicals randomly selected from IASJ website related to corrosion inhibitor and introduced in free online Biosig –Lab/ tool website [15, 17, 18] to get knowledge about their effects on foetus's health (teratogenic risk [17]), cardiac [18]: Arrhythmia, Cardiac Failure, Heart Block, hERG toxicity, Hypertension, and Myocardial Infarction beside honey bee (*A. mellifera*), *mallard* and *flathead minnow*, human health: AMES, rat LD_{50} and oral chronic toxicities [15] as shown in Figure (1).

2. Experimental Section

2.1. Chemicals

Seven chemicals varied in their structures were chosen (Table 1 & Figure 2) with their general information that mentioned in their references.

Table (1): Selected corrosion inhibitors for toxicity prediction in their references.

ID	Compound name (general or specific)	SMILES	Corrosive medium	General experimental information	Ref.
CHAB	Aromatic Schiff base linked to azo, 4-(((3-((4-acetylphenyl) diazenyl)-2-hydroxynaphthalen-1-yl) methylene) amino) benzoic acid	OC(=O)C1=CC=C(C=C1)\N=C/C1=C2C=CC=CC2=CC=C1\N=N\C1=CC=C(C=C1)C(O)=O	1M HCl	carbon steel, (0.1, 0.5, 1 and 5) mM, (298-318) K, Potentiodynamic polarization, inhibition efficiency: 94.77% at 5 mM at 298 K, Langmuir isotherm,	19
TEOSDEOP	Tri-ethoxysilyl-di-ethylphosphate	CCO[Si](CCP(=O)(OCC)OCC)(OCC)OCC	1M HCl, distilled water sea water tap water	carbon steel alloy A36, weight loss and electrochemical methods. inhibition efficiencies: 99.19% for 10 ppm, 98.35% for 20 ppm in distilled, tap and seawater, respectively, 97.65% for 30 and 40ppm in HCl.	20
Tz	di (1-butyl tetrazole-5-yl) tellurium dibromide	CCCCN1N=NN=C1[Te](Br)(Br)C1=NN=NN1CCCC	1M HCl	carbon steel alloys, (303, 313 and 323) K, (5, 10 and 30) ppm. Polarization, inhibition efficiency 87% at 30 ppm and 303 K.	21
N-2-M	Carnosine	C1=C(NC=N1)CC(C(=O)O)NC(=O)CCN	1M HCl	mild steel , 30ºC, Weight loss, inhibition efficiency: 91%.	22
HYD	6-chloro-1,1-dioxo-3,4-dihydro-2H-1λ6,2,4-benzothiadiazine-7-sulfonamide [Hydrochlorothiazoide]	C1NC2=CC(=C(C=C2S(=O)(=O)N1)S(=O)(=O)N)Cl	1M HCl	Aluminum 7075, (35 and 55) °C, weight loss, Langmuir isotherm, Quantum chemical calculations: DFT, B3YLP and 6-311++G (d ,p).	23

ID	Compound name (general or specific)	SMILES	Corrosive medium	General experimental information	Ref.
AND	2-amino-4-(4-nitrophenyl)-3-cyano-4, 5-dihydropyrano (3,2-c) coumarin	NC1=C(C#N)C(C2=CC=C(C=C2)[N+](O)=O)C2=C(O1)C1=C(OC2=O)C=CC=C1	1M HCl	Mild steel, weight loss, inhibition performance: 96%	24
Thoron	o-arsono-phenylazo-2-naphthol-3,6-disulfonic acid sodium salt	C1=CC=C(C(=C1)N=NC2=C3C=CC(=CC3=CC(=C2O)S(=O)(=O)[O-])S(=O)(=O)[O-])[As](=O)(O)O.[Na+].[Na+]	1M HCl and 1M H2SO4	weight loss, potentiodynamic polarization, and quantum chemical calculations. Weight loss: (1-4) hrs., (298 to 318) K, C-steel, efficiency: 91.99% at 0.001M at 298 K. Potentiodynamic polarization: efficiency: 93.74% same conditions. Langmuir adsorption isotherm was tested.	25

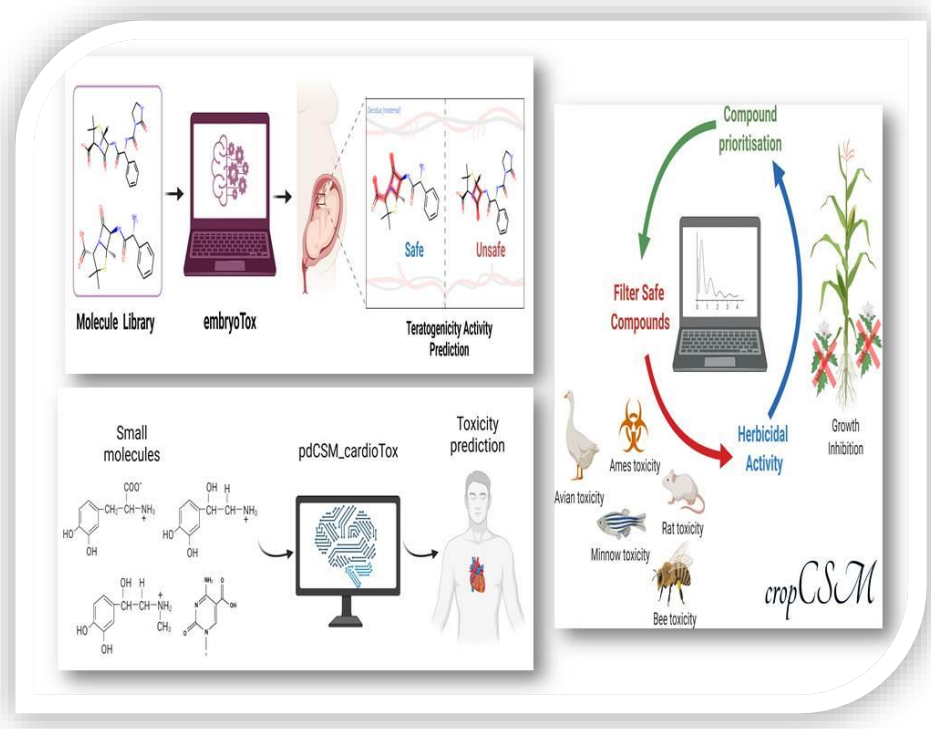

Figure (1): Representative diagram about toxicity prediction [15, 17, 18].

2.2. *In Silico* – Online Prediction

These seven materials (Table 1 & Figure 2) were drawn by ChemDraw Pro 8.0 then converted to "Simplified Molecular Input Line Entry System, SMILES" as a translation of its three-dimensional structure into a string of symbols by MarvinSketch program. These smiles can be understood by online website software. Each SMILES symbol was introduced in free online Biosig –Lab/ tool website [15, 17, 18] to predict:

a. Embro-toxicity or foetus's health (teratogenic risk) [15],
b. Arrhythmia, Cardiac Failure, Heart Block, hERG toxicity, Hypertension, and Myocardial Infarction as Cardio-toxicity [17],
c. and crop-toxicity of honey bee (A. mellifera), mallard and flathead minnow, human health: AMES, rat LD50 and oral chronic toxicities [18].

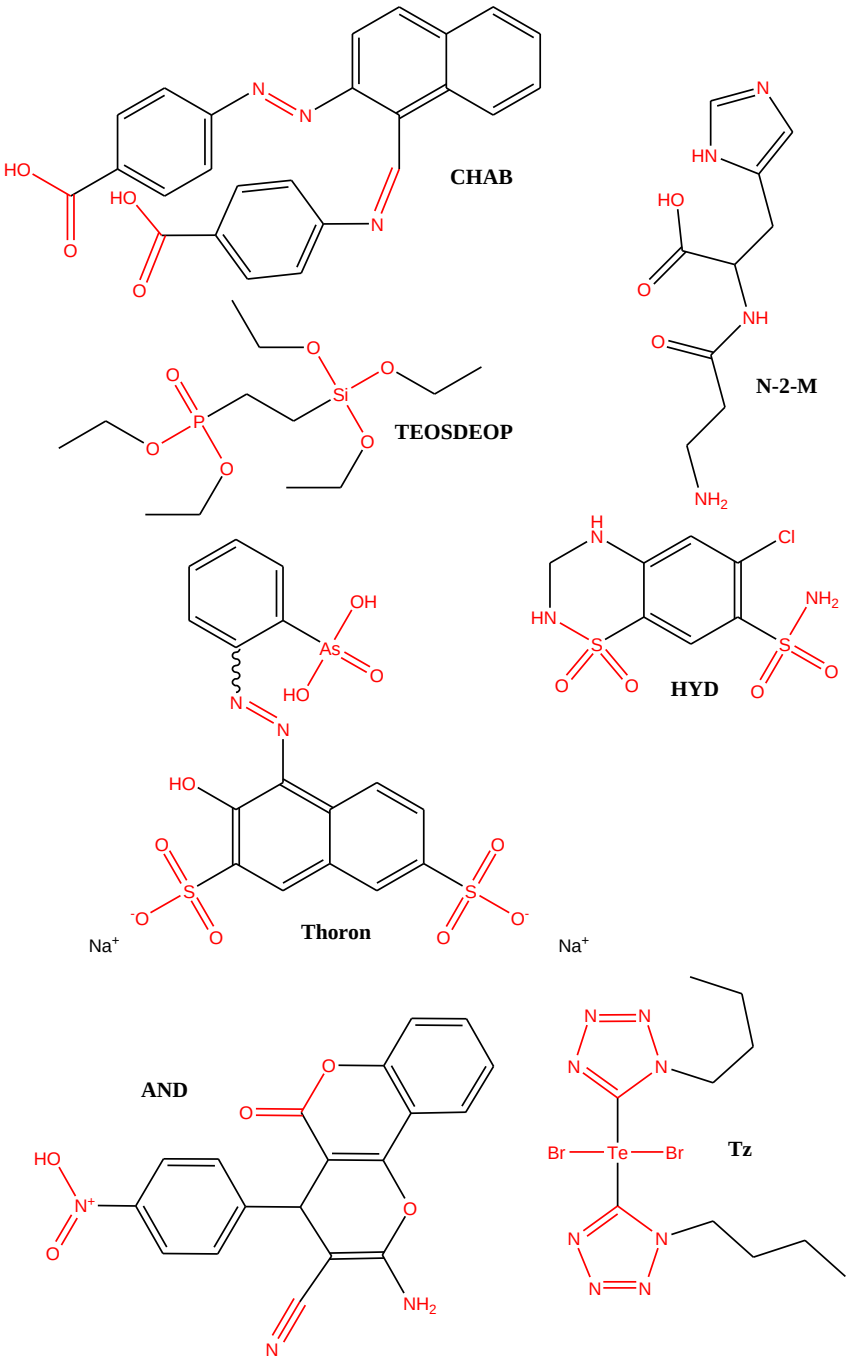

Figure (2): Chemical structures of the tested corrosion inhibitors.

Table (2a): *In Silico* prediction results of the selected corrosion inhibitors.

ID	Embro-toxicity		Cardio- toxicity					
	Safety profile	**Confidence level**	***Arrhythmia***	***Cardiac Failure***	***Heart Block***	***hERG Toxicity***	***Hypertension***	***Myocardial Infarction***
CHAB	**Unsafe**	High	Safe	**Toxic**	Safe	Safe	Safe	Safe
TEOSDEOP	**Unsafe**	High	Safe					
Tz	**Unsafe**	High	Safe	Safe	Safe	Safe	**Toxic**	Safe
N-2-M	**Unsafe**	Medium	Safe					
HYD	**Unsafe**	High	Safe	Safe	Safe	Safe	**Toxic**	Safe
AND	**Unsafe**	High	Safe					
Thoron	**Unsafe**	Medium	Safe	Safe	Safe	**Toxic**	Safe	Safe

Table (2b): *In Silico* prediction results of the selected corrosion inhibitors.

ID	Herbicidal Activity	Environmental Toxicity			Human toxicity		
	Herbicide Activity	***Honey Bee Toxicity***	***Avian Toxicity***	***Minnow Toxicity***	***AMES Toxicity***	***Rat Acute Toxicity (LD_{50})***	***Rat Chronic Toxicity (LOAEL)***
CHAB	No	No	No	-0.875	**Yes**	1858.9	19.1
TEOSDEOP	No	No	No	1.262	No	86.4	3.1
Tz	No	**Yes**	**Yes**	2.205	No	540.3	10.9
N-2-M	No	No	No	2.56	No	1962.9	26.1
HYD	No	No	No	2.421	No	3155.3	6.9
AND	No	**Yes**	No	0.468	**Yes**	486.7	88.6
Thoron	No	No	No	1.957	No	2436.1	3.3

3. Results and Discussion

In metal or non-metallic protection topics, organic inhibitors are widely subjected in both coating and solution states looking for effectiveness and economic protection. These substances may contain heteroatoms in their molecular structure such as (N, O, P, metal, halide, …) as well as aromatic ring, double or triple bond as a source of π- electronic cloud. According to available literatures, these materials considered as a base for physical or chemical adsorption layer(s) formed at the metal surface then inhibited with cathodic / anodic reaction in the electrochemical medium. Exploring the ability of organic interfaces with metal base is greatly attracted with environmental limitations such as biodegradability, toxicity, solubility, …etc. and requested a high performance especially in such a complex phenomenon. Molecular structure, pH, temperature, concentration, and others are controlling factors in inhibition and adsorption steps [1, 2, 3, 26, 27, 28].

Computational modeling has extensively investigated corrosion inhibition by various theoretical simulations like Density Functional Theory (DFT), Monte Carlo, and others to recognize how organic species interact with surface (mimic approach). Online in Silico investigation is a computational based method utilized for QSAR – ADMET prediction of organic or organo- metallic compounds.

Here, a new attempt to predict toxicity of seven chemicals used as corrosion inhibitors by Iraqi researchers in Iraqi academic journals (Tables 1 & 2, Figure 2). Prediction sets a remarkable toxicity notes such as:

- All studied compounds were moderate to extremely unsafe to the health of foetus during pregnancy. So, they may be considered as a teratogen if the pregnant ingested or exposed with extraordinary fetal risk for example preterm labor, miscarriage, or stillbirth.
- CHAB, Tz, HYD, and Thoron had various cardio- toxicological states. Tz and HYD may causes hypertension.
- All tested materials have No response to herbicidal activity but Tz & AND were toxic to honey bee (A. mellifera).
- All materials under investigation were safe to avian except Tz.
- Only CHAB can be counted as safe to fish (mallard and flathead minnow).
- CHAB & AND were toxic in Ames testing or Salmonella typhimurium reverse mutation assay. So, they can cause DNA mutation of this tested bacterium meaning they were identified as carcinogenic materials.
- LD_{50} range was 86.4 to 3155.3 while LOAEL was 3.1 to 88.6 where TEOSDEOP had the minimum acute and chronic toxicity to rat.
- This TEOSDEOP had the minimum toxicological results while Tz had the maximum foundation between chemicals under in Silico – online website assessment.
- Final conclusion, all tested corrosion inhibitors were structurally unsafe to human and/or environment.

4. Conclusions

First Iraqi attempt to evaluate toxicity of corrosion inhibitors to human and environment was done with the assistance of online websites – mathematical based approach. Embro-toxicity, Cardio-toxicity, and crop-toxicity were screened by the tested toxicological web servers in this attempt. Seven corrosion inhibitors varied in their

chemical structures were selected from Iraqi journals and tested by these online websites. As stated by these *in Silico* prediction testing, all tested corrosion inhibitors were structurally unsafe to human and/or environment.

Conflict of Interest: The authors declare that there are no conflicts of interest associated with this research project. We have no financial or personal relationships that could potentially bias our work or influence the interpretation of the results.

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