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REVIEWER'S REPORT

Manuscript No.: **IJAR-54149** **Date**: 02-10-2025

Title: QUANTUM CHEMICAL AND KINETIC PROPERTIES EVALUATION OF METHYLCHROMENO[2,3-C]PYRAZOL-3(2H)-ONE FOR ALUMINUM CORROSION INHIBITION IN H_2 S0_4 MEDIUM

Recommendation:
Accept as it is .....
Accept after minor revision .....✓.....
Accept after major revision.....
Do not accept (*Reasons below*) .....

Rating	Excel.	Good	Fair	Poor
Originality		✓		
Techn. Quality		✓		
Clarity			✓	
Significance			✓	

Reviewer Name: **Sudhanshu Sekhar Tripathy** **Date:** 02-10-2025

Reviewer's Comment for Publication.

(*To be published with the manuscript in the journal*)

The reviewer is requested to provide a brief comment (3-4 lines) highlighting the significance, strengths, or key insights of the manuscript. This comment will be Displayed in the journal publication alongside with the reviewer's name.

Reviewer's Comment for Publication

The manuscript presents an experimental and computational evaluation of **2-methylchromeno[2,3-c]pyrazol-3(2H)-one (MCP)** as an inhibitor for aluminum corrosion in **sulfuric acid medium**. It combines **gravimetric measurements and Density Functional Theory (DFT) calculations**, making it a strong interdisciplinary contribution to **corrosion science, quantum chemistry, and materials engineering**. The results confirm the inhibitor's high efficiency (up to 92.87%) and provide insights into adsorption mechanisms. The study is well-written and scientifically significant but requires **minor revisions** for refinement of methodology description, reference formatting, and clarity in presentation.

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Detailed Reviewer's Report

1. Scope & Relevance:

- Highly relevant to **corrosion inhibition, materials protection, and quantum chemical modeling**.
- Provides both practical (industrial corrosion mitigation) and theoretical (DFT insights) contributions.

2. Structure & Technical Presentation:

- The paper follows a standard format: Abstract, Introduction, Methods, Results, Discussion, and Conclusion.
- Figures and tables are informative (molecular structure, optimized geometry, inhibition efficiency graphs).
- Suggested improvement: add a **schematic flowchart of experimental + computational workflow** to improve clarity.

3. Experimental / Methodological Details:

- Gravimetric method and DFT calculations are well described.
- Improvements needed:
  - Specify the **number of experimental repeats** and error margins for measurements.
  - Clarify **boundary conditions** in DFT simulations (e.g., solvent model, convergence criteria).
  - Discuss limitations such as **temperature range applicability** and **industrial scaling challenges**.

4. References & Citations:

- References include both classical and recent works (2015–2024).
- Issues:
  - Some references are not formatted consistently (capitalization, punctuation, journal titles).
  - Add **more recent sources (2022–2025)** on green inhibitors, DFT corrosion studies, and sustainable materials protection.
  - Ensure uniform referencing style as per IJAR guidelines.

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5. Language & Style:

- Clear scientific language with good readability.
- Minor grammatical issues (verb tense, article usage) should be corrected.
- Ensure consistency in chemical terms (e.g., *physiosorption* → *physisorption*).

6. Key Strengths:

- Combination of **experimental validation and theoretical modeling**.
- Strong correlation between **gravimetric results and DFT descriptors**.
- Practical relevance in **industrial corrosion prevention strategies**.

7. Areas for Improvement:

- Include a **flowchart of the methodology** (gravimetric + DFT steps).
- Add details on **experimental error margins and repeatability**.
- Expand references with **newer studies** (2022–2025).
- Minor language polishing required.

Final Feedback to Author

This is a **valuable contribution to corrosion science and quantum chemical modeling**. With **minor revisions** in methodology detail, references, and presentation style, the manuscript will be ready for publication.