**Exploring Sustainable Corrosion Inhibition of Copper in Saline Environment: An Examination of Hydroquinazolinones via Experimental and ab initio DFT simulations**

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***S1. Synthesis of compounds***

***1-((4-hydroxynaphthalen-1-yl)methyl)-2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (DQ-CH3):***

Chemical Formula: C26H22N2O2

Molecular Weight: 394.47



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Fig.S1. Spectral 13 C and 1 H NMR for compound DQ-CH3.

***1-((4-hydroxynaphthalen-1-yl)methyl)-2-phenyl-2,3-dihydroquinazolin-4(1H)-one (DQ-H):***

Chemical Formula: C25H20N2O2

Molecular Weight: 380,44



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**Fig.S2.** Spectral 13 C and 1 H NMR for compound DQH.

**Table S2.** Fukui function indices of DQ-CH3 and DQ-H compounds obtained by DFT/GGA.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| DQ-CH3 | Fukui(+) | Fukui(-) | DQ-H | Fukui(+) | Fukui(-) |
| C ( 1) | 0.026 | 0.034 | C ( 1) | 0.034 | 0.026 |
| C ( 2) | 0.025 | 0.034 | C ( 2) | 0.034 | 0.024 |
| C ( 3) | 0.021 | 0.023 | C ( 3) | 0.022 | 0.021 |
| C ( 4) | 0.018 | 0.033 | C ( 4) | 0.031 | 0.017 |
| C ( 5) | 0.013 | 0.012 | C ( 5) | 0.012 | 0.012 |
| C ( 6) | 0.015 | 0.014 | C ( 6) | 0.014 | 0.014 |
| C ( 7) | 0.036 | 0.023 | C ( 7) | 0.022 | 0.036 |
| C ( 8) | 0.028 | 0.024 | C ( 8) | 0.023 | 0.027 |
| C ( 9) | 0.031 | 0.022 | C ( 9) | 0.022 | 0.031 |
| C ( 10) | 0.035 | 0.022 | C ( 10) | 0.021 | 0.034 |
| O ( 11) | 0.018 | 0.039 | O ( 11) | 0.038 | 0.018 |
| C ( 12) | 0.007 | 0.014 | C ( 12) | 0.014 | 0.007 |
| N ( 13) | 0.009 | 0.065 | N ( 13) | 0.066 | 0.009 |
| C ( 14) | 0.023 | 0.023 | C ( 14) | 0.024 | 0.023 |
| C ( 15) | 0.033 | 0.038 | C ( 15) | 0.039 | 0.033 |
| C ( 16) | **0.054** | 0.013 | C ( 16) | 0.014 | 0.054 |
| N ( 17) | 0.030 | 0.015 | N ( 17) | 0.015 | 0.030 |
| C ( 18) | 0.009 | 0.011 | C ( 18) | 0.011 | 0.009 |
| C ( 19) | 0.048 | 0.035 | C ( 19) | 0.035 | 0.048 |
| C ( 20) | 0.033 | 0.069 | C ( 20) | 0.070 | 0.033 |
| C ( 21) | 0.061 | 0.035 | C ( 21) | 0.036 | 0.061 |
| C ( 22) | 0.032 | 0.046 | C ( 22) | 0.047 | 0.032 |
| O ( 23) | 0.067 | 0.031 | O ( 23) | 0.031 | 0.067 |
| C ( 24) | 0.005 | 0.003 | C ( 24) | 0.003 | 0.007 |
| C ( 25) | 0.011 | 0.005 | C ( 25) | 0.005 | 0.012 |
| C ( 26) | 0.009 | 0.009 | C ( 26) | 0.009 | 0.011 |
| C ( 27) | 0.013 | 0.009 | C ( 27) | 0.011 | 0.018 |
| C ( 28) | 0.011 | 0.009 | C ( 28) | 0.009 | 0.013 |
| C ( 29) | 0.010 | 0.009 | C ( 29) | 0.009 | 0.012 |
| C ( 30) | 0.004 | 0.003 |  |  |  |

**Table S3:** Comparative chart listing performances of some other quinazolines and quinazolinones acting as corrosion inhibitors of various metals.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Inhibitor structure** | **Metal/solution** | **Techniques** | **Efficiency at max. concentration** | **Ref.** |
| **DQ-Br**    **DQ-Cl**    **DQ-Cl’** | Copper/NaCl | EIS, PDP, WL, SEM, FT-IR, UV-vis, DFT, MD | **DQ-Br**: 97.24%  **DQ-Cl**: 95.24%  **DQ-Cl’**: 94.18% | (Oubahou et al., 2023) |
| **PPQ**    **MPPQ** | Mild Steel/1M HCl | Mass loss, PDP EIS, SEM/EDS, XPS, AFM, DFT, MD | **PPQ** : 95.7%  **MPPQ** : 95.2% | (W. Chen et al., 2021b) |
| **QZ-H**    **QZ-OH**    **QZ-CH3**    **QZ-NO2** | Mild Steel/1M HCl | PDP, EIS, SEM, UV-visible, DFT, MC | **QZCH3**: 96.52%  **QZ-OH**: 93.13%  **QZ-NO2**: 90.74%  **QZ-H**: 85.37% | (Errahmany et al., 2020) |
| **HQ-ZH**    **HQ-ZNO2**    **HQ-ZOH** | Mild steel/1M HCl | PDP, EIS, SEM, UV-visible, DFT,  Monte Carlo simulations | **HQ-ZNO2**: 95.9%  **HQ-ZH**: 94.4%  **HQ- ZOH**: 91.4% | (Rbaa, Galai, et al., 2019) |
| **DM**    **DME** | Copper/0.5M H2SO4 | PDP, EIS, SEM, AFM, XPS, FT-IR, DFT, MD | **DME**: 88.1%  **DM**: 86.0% | (J. Zhang & Zhang, 2021) |
| **BQA**    **QA**    **HQA**    **ThQA**    **SHQA** | COPPER/ HNO3 | Gravimetry, electrochemical | **SHQA**: 58.9%  **ThQA**: 52.0%  **HQA**: 50.4%  **QA**: 45.0%  **BQA**: 42.0% | (A. E.-A. S. Fouda et al., 2010) |
| **PDQ** | MS/0.1M HCl | EIS, PDP, Quantum chemical | 92.93 % | (Ayati et al., 2011) |
| **Metolazone** | Mild steel/HCl | WL, electrochemical, SEM, DFT | 82.8% | (Arrousse et al., 2022) |
| **(1)**    **(2)**    **(3)** | Carbon steel/2M HCl | WL, PDP, EIS, EDS, SEM | **(1)**: 75.4%  **(2)**: 59.8%  **(3)**: 49.8% | (A. S. Fouda & Hassan, 2013) |
| **HMPB**    **BHMB** | Carbon steel/1M HCl | WL, PDP, EIS, UV-vis, DFT | **BHMB :** : 86.7%  **HMPB :** 81.6% | (Faydy et al., 2019) |
| **Q1**    **Q2**    **Q3** | MS/0.5M HCl | EIS PDP SEM DFT | **Q1**: 95.3%  **Q2** : 90.1%  **Q3** : 86.2% | (Kumar et al., 2020) |
| **MMDQ**    **NNDQ** | Mild stel/1M HCl | Mass loss, OCP, PDP, EIS, SEM | **MMDQ** : 92%  **NNDQ** : 89% | (G. Khan et al., 2017) |
| **Q1A**    **Q1B**    **Q1C** | Mild steel/H2SO4 | DFT, MD | **Q1A**: 96%  **Q1B**: 89%  **Q1C**: 50% | (Saha et al., 2016) |
| **QZ-H**    **QZ-Cl** | Mild steel/1M HCl | PDP, EIS, DFT | **QZ-Cl**: 88.62%  **QZ-H**: 86.20% | (Touir et al., 2024) |
| **QDO**    **QIM** | Mild steel/1M HCl | PDP, EIS, SEM/EDS, UV-vis, FT-IR, DFT | **QIM**: 97.95%  **QDO**: 92.59% | (Rbaa & Lakhrissi, 2019) |
| **DHIP1**    **DHIP2** | Low Alloy Steel/ HCl | Weightloss, Electrochemical, SEM | **DHIP1** : 86.3%  **DHIP2** : 81.8% | (G. Khan et al., 2018) |