**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







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







**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) |