CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2025, 20(2), 84-93
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
https://doi.org/10.19261/cjm.2025.1342

EMPLOYMENT OF *IN SILICO* IN PREDICTION OF FURAN DERIVATIVES AS EFFICIENT CORROSION INHIBITORS FOR MILD STEEL IN ACIDIC MEDIA

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Abstract. This study highlights the role of computational approaches in advancing the design of corrosion inhibitors by virtually screening novel candidate molecules. In silico treatment based on quantitative structure-activity relationship (QSAR) analysis was performed on already published experimental results of corrosion inhibition efficiency (IE%) of mild steel in acidic media for eighteen furan derivatives. The theoretical treatments are based on density functional theory (DFT) at B3LYP level. It was found that the global minimum of the furan derivatives can be reached at a medium basis set of 6–21G. A sophisticated model consisting of four descriptors excluding the sulphur correction term with physical meaning and good statistical criteria of squared correlation coefficient (r^2) and standard error (SE) equal to 0.914 and 5.029, respectively, is presented. The suggested model can be considered as a powerful tool for understanding the role of chemical composition in preventing corrosion which helps researchers in the development process. The *in silico* treatment was utilized for suggesting twelve furan derivatives with an extremely high IE% which might be used as excellent materials for corrosion inhibition when synthesized and applied experimentally.

Keywords: furan derivative, *in silico*, corrosion inhibitor, mild steel, density functional theory.

Received: 25 July 2025/ Revised final: 07 November 2025/ Accepted: 10 November 2025