

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

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Abstract. This research deals with the contribution of *in silico* analysis in the development of corrosion inhibitors field by predicting adequate new molecules that could be employed for this purpose. A quantitative structure-activity relationship (QSAR) analysis of already published experimental results of corrosion inhibition efficiency (IE%) of mild steel in acidic media for eighteen furan derivatives was performed. 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. 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.