## LIST OF ABBREVIATIONS USED IN THE THESIS

| | | |
|---|---|---|
| DS | : | Derivative Spectrophotometry |
| SD | : | Standard deviation |
| σ | : | Standard deviation of the reagent blank |
| D | : | Density |
| RSD | : | Relative standard deviation |
| $Q_L$ | : | Quantitation limit |
| $D_L$ | : | Detection limit |
| ETU | : | Ethylene Thiourea |
| DFT | : | Density functional theory |
| TG | : | Thermogravimetry |
| DTA | : | Differential Thermal Analysis |
| IR | : | Infra Red |
| UV | : | Ultra Violet |
| NMR | : | Nuclear Magnetic Resonance |
| ESR | : | Electron Spin Resonance |
| TCNE | : | Tetracyanoethylene |
| VOIP | : | Valence orbital ionization potential |
| ADME | : | Absorption, distribution, metabolism and elimination |
| HIA | : | Human intestinal absorption |
| BBB | : | Blood-Brain Barrier |
| MM | : | Molecular mechanics |
| SE | : | Semi empirical calculations |
| HEMTDT | : | (E)-4-(2-hydroxyphenyl) ethylideneamino)-6-methyl-3-thioxo-3, 4-dihydro-1, 2, 4-triazin-5(2H)-one |
| CBMTDT | : | (E)-4-(2-chlorobenzylideneamino)-6- methyl-3-thioxo-3, 4-dihydro-1, 2, 4-triazin-5(2H)-one |

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|---|---|---|
| MMTDT | : | (E)-4-(4-methoxybenzylideneamino)-6-methyl-3-thioxo-3, 4-dihydro-1, 2, 4-triazin-5(2H)-one |
| DMSO | : | Dimethyl sulfoxide |
| DMF | : | Dimethyl formamide |
| V.P.I | : | Vapor phase inhibitor |
| SAM | : | Self-assembled monolayer |
| OCP | : | Open Circuit Potential |
| EIS | : | Electrochemical impedance spectroscopy |
| LPR | : | Linear Polarization Resistance |
| B3LYP | : | Becke 3 Lee-Yang-Parr |
| MBATD | : | (E)-(4-(4-methoxybenzylideneamino)-4H-1, 2, 4-triazole-3, 5-diyl) dimethanol |
| IE | : | Inhibition efficiency |
| PMMA | : | Polymethylmethacrylate |
| MS | : | Mild Steel |
| SCE | : | Saturated calomel electrode |
| $R_{ct}$ | : | Charge transfer resistance |
| $C_{dl}$ | : | Double layer capacitance |
| $i_{corr}$ | : | Corrosion current density |
| $K_{ads}$ | : | Equilibrium constant of the adsorption process |
| $E_{corr}$ | : | Corrosion potential |
| $\beta_a$ | : | Anodic Tafel slope |
| $\beta_c$ | : | Cathodic Tafel slope |
| HOMO | : | Highest Occupied Molecular Orbital |
| LUMO | : | Lowest Unoccupied Molecular Orbital |
| EDAX | : | Energy dispersive x-ray |
| SEM | : | Scanning Electron microscopy |

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|---|---|---|
| $\Delta S^{0}_{ads}$ | : | Entropy of Adsorption |
| $\Delta H^{0}_{ads}$ | : | Enthalpy of adsorption |
| $\Delta G^{o}_{ads}$ | : | Free energy of adsorption |
| $E_{total}$ | : | The total energy |
| $E_{rigid\ adsorption}$ | : | Rigid adsorption energy |
| $E_{deformation}$ | : | Deformation energy |
| A | : | Electron affinity |
| I | : | Ionization potential |
| $\chi_M$ | : | The absolute electro negativity of metal |
| $\chi_{inh}$ | : | The absolute electro negativity of the inhibitor molecule |
| $\eta_M$ | : | The absolute hardness of metal |
| $\eta_{inh}$ | : | The absolute hardness of inhibitor molecules |
| $\Delta N$ | : | The number of electrons transferred |
| a.c | : | Alternating current |
| k | : | Equilibrium constant |
| R | : | Gas constant |
| T | : | Temperature |
| t | : | Time |
| f+ | : | Site for nucleophilic attack |
| f- | : | Site for electroucleophilic attack |