A detailed investigation on the anticorrosive performance of the newly synthesized imidazole derivatives MBI, BIDM and TITM on mild steel in ground water medium was carried out. Synthesis of the three imidazole derivatives 1-(4-methoxybenzyl)-1H-imidazole (MBI), 1,4-bis(N-imidazolylmethyl)-2-5-dimethoxybenzene (BIDM) and 1,3,5-tris(N-imidazolylmethyl)-2,4,6-trimethoxybenzene (TITM) was carried out in the laboratory by adopting simple synthetic route. The corrosion inhibition of mild steel in ground water medium has been investigated using the newly synthesized inhibitors MBI, BIDM and TITM by employing gravimetric analysis, potentiodynamic polarization and electrochemical impedance spectroscopy techniques. In addition morphology of the mild steel specimens were pictured and discussed with the SEM and AFM techniques. All these results were further substantiated with the density function theory calculation. By assessing the results of gravimetric as well as electrochemical techniques along with quantum chemical calculation, the following conclusions were drawn:

1. The purity and formation of the as-synthesized three new imidazole derivatives MBI, BIDM and TITM have been confirmed using $^1$H-NMR and $^{13}$C-NMR techniques.
2. All the three imidazole derivatives acted as good corrosion inhibitors for mild steel corrosion in ground water media and the corrosion inhibition efficiency increased with increasing inhibitor concentration for both the weight loss measurements as well as electrochemical characterizations.

3. The variation in inhibition efficiency mainly depends on the nature of the substituent present in the inhibitor molecules. The increase in number of substituent increases the block active sites and hence the inhibition efficiency is higher for TITM. The inhibition efficiencies of these compounds determined by the gravimetric analysis and electrochemical techniques are in good agreement and their obtained inhibition efficiencies are in the order of MBI<BIDM<TITM.

4. The evaluation of polarisation measurements using these compounds revealed the inhibition of both anodic and cathodic reaction by adsorption on the mild steel surface thereby act as mixed type inhibitors.

5. Among the newly synthesised single podal, bipodal and tripodal structured imidazole derivatives, TITM (tripodal) provided an increased corrosion inhibition efficiency of 90% than that of BIDM (80%) and MBI (70%) at their optimum concentrations say 1.01 mM, 0.67 mM and 0.49 mM, respectively which could be revealed by the experimental techniques like weight loss, polarisation and impedance for mild steel corrosion in ground water medium.
6. Quantum chemical data obtained from 6-31*G basis set such as HOMO, LUMO, \( \chi \) and \( \Delta E \) shows that among the newly synthesized imidazole derivatives, TITM adequately inhibits mild steel corrosion in ground water medium.

7. The as-predicted structure and molecular suitability of MBI, BIDM and TITM confirm that the inhibition is due to adsorption. Also the adsorption of inhibitor molecules on mild steel surface obeys the Langmuir adsorption isotherm.

8. The results obtained from the morphological investigations showed that the mild steel is protected against corrosion and its deterioration on its surface by the adsorption of the inhibitor molecules which stands as a protective barrier against the invasion of corrosive ions.

9. The investigation on the inhibitory performance at different temperatures 30, 40, 50 and 60\(^\circ\)C clearly evidenced the decrease of inhibition efficiency while increasing the temperature. It is also observed that among the three imidazoles, TITM possessed higher activation energy.

10. Finally, this study shows a good correlation between the theoretical and experimental data which confirms the reliability of quantum chemical methods to study the inhibition of corrosion of metal surfaces in order to be deployed in future industrial purpose against corrosion in water storage tanks, pipelines, cooling tower systems etc.