**ABSTRACT**

Novel Substituted 4′-methyl-3-thioxo-1,2,4-triazinoquinoline-5-ones are subjected to the anti bacterial and antifungal studies. Density Functional theory calculations of the compounds were performed using molecular structures with optimized geometries. The optimized geometry of the compounds were obtained by using 6-31G (d,p) basis set, and the Frontier Orbital energy and electrostatic potential were interpreted. The structureactivity relationships between the theoretical and wet lab results were discussed. All the products were screened in vitro antibacterial and antifungal activity against different micro organisms.