

**VIRTUAL SCREENING, MOLECULAR DOCKING STUDIES,
ADMET PROPERTIES, DENSITY FUNCTIONAL THEORY AND
2D-QSAR MODELING TO DESIGN POTENTIAL INHIBITORS**

*A Thesis submitted to the University of North Bengal
For the Award of
Doctor of Philosophy
in
Chemistry*

By

SUBHAJIT SARKAR

SUPERVISOR

Dr. Rajesh Kumar Das

**Department of Chemistry
University of North Bengal
January, 2023**