In Silico Novel Identification of Anti-cancer Drugs using Density Functional Theory and Molecular Dynamics Simulation

A THESIS

SUBMITTED TO THE MAHARAJA SAYAJIRAO UNIVERSITY OF BARODA

FOR THE AWARD OF THE DEGREE OF

Doctor of Philosophy

Physics

BY Ms. Anjali Patel



Under the supervision of

Prof. Prafulla K. Jha

Department of Physics, Faculty of Science The Maharaja Sayajirao University of Baroda Vadodara – 390 002, India

November 27, 2020