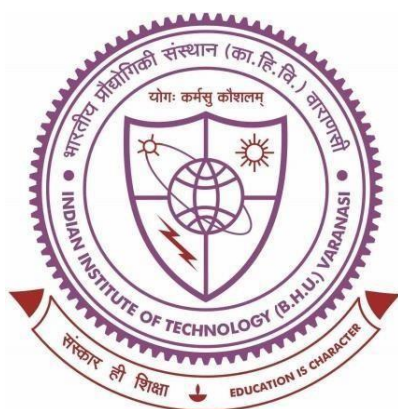


**DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF
NOVEL PROTEIN AGGREGATION MODULATORS AS
POTENTIAL THERAPEUTICS AGAINST ALZHEIMER'S
DISEASE**



Thesis submitted in partial fulfillment
for the Award of Degree

Doctor of Philosophy

By

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Dedicated to my family

CERTIFICATE

It is certified that the work contained in the thesis titled “**Design, Synthesis, and Biological Evaluation of Novel Protein Aggregation Modulators as Potential Therapeutics Against Alzheimer’s Disease**” by **Bhanuranjan Das** has been carried out under my supervision and that this work has been not submitted elsewhere for a degree.

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LIST OF ABBREVIATIONS

Abbreviation	Full form
Ach	Acetylcholine
AD	Alzheimer's Disease
ADME	Absorption, Distribution, Metabolism and Excretion
ADT	AutoDock Tools
AI	Artificial Intelligence
ANOVA	Analysis of Variance
APP	amyloid precursor protein
ATR-FTIR	Attenuated Total Reflection- Fourier Transform Infrared Spectroscopy
A β	Amyloid Beta
BBB	Blood Brain Barrier
CADD	computer aided drug design
ChAT	Choline Acetyltransferase
CNS	Central Nervous System
DCM	Dichloromethane
De	External Distance
DFT	Density Functional Theory
Di	Internal Distance
DL	Deep Learning
DMSO	Dimethyl Sulfoxide
DNP	Donepezil
DPPH	2,2 Diphenyl-1-Picrylhydrazyl
DruMAP	Drug Metabolism And Pharmacokinetics Analysis Platform
ECFP	Extended-Connectivity Fingerprint
EGCG	Epigallocatechin-3-Gallate
EPM	Elevated Plus Maze
FDA	Food And Drug Administration
FEL	Free Energy Landscape
FMOs	Frontier Molecular Orbitals
FP	Fingerprint Plot
FT-IR	Fourier-Transform Infrared Spectroscopy
GIAO	Gaussian With Gauge Independent Atomic Orbital
GROMACS	Groningen Machine For Chemical Simulation
GSK-3 β	Glycogen Synthase Kinase-3
HBA	Hydrogen Bond Acceptor
HBD	Hydrogen Bond Distance
HBD	Hydrogen Bond Donor
HFIP	Hexafluoroisopropanol
HIV-1	Human Immunodeficiency Virus-1
HOMO-	Highest Occupied Molecular Orbital-
LUMO	Lowest Unoccupied Molecular Orbital
HRMS	High Resolution Mass Spectroscopy

Abbreviation	Full form
HS	Hirshfeld Surface
I3C	Indole-3-Carbinol
IAA	Indole-3-Acetic Acid
IDO	Indoleamine 2,3-Dioxygenase
IR	Infra-Red Spectroscopy
spectroscopy	
LBDD	Ligand Based Drug Design
LED	Light-Emitting Diode
MAPT	Microtubule-Associated Tau Protein
MD	Molecular Dynamics
MEP	Molecular Electrostatic Potential
MHFP	Minhash Fingerprint
ML	Machine Learning
MMPBSA	Molecular Mechanics Poisson-Boltzmann Surface Area
MPA	Mulliken Population Analysis
MW	Molecular Weight
NBO	Natural Bond Orbital
NFTs	Neurofibrillary Tangles
NMDA	N-Methyl D-Aspartate
NMR	Nuclear Magnetic Resonance
PAINS	Pan Assay Interference Compound
PAMPA	Parallel Artificial Membrane Permeability Assay
PBS	Phosphate Buffer Saline
PCA	Principal Component Analysis
PHFs	Paired Helical Filaments
PL Inhibition Assay	Pancreatic Lipase Inhibition Assay
PMF	Potential of Mean Force
PyRMD	Python Based Random Matrix Discrimination
QSAR	Quantitative Structure Activity Relationship
REMD	Replica Exchange Molecular Dynamics
RMSD	Root Mean Square Deviation
RMSF	Root Mean Square Fluctuation
RoG	Radius Of Gyration
ROS	Reactive Oxygen Species
SBDD	Structure Based Drug Design
SDS	Sodium Dodecyl Sulphate
SEM	Standard Error Of Mean
SMILES	Simplified Molecular Input Line Entry System
TD-DFT	Time Dependent Density Functional Theory
THF	Tetrahydrofuran
Th-T	Thioflavin-T
TMS	Tetramethylsilane

Abbreviation	Full form
TPSA	Topological Polar Surface Area
TTR	Transthyretin
USFDA	United States Food And Drug Administration
vdW	van der Waals
WHO	World Health Organization
XRD	X-Ray Diffraction
