

CERTIFICATE

This is to certify that the thesis entitled “**Inverse Electron Demand Diels Alder Reaction of Pyrido[1,2-*a*]pyrimidine-2-ones - Experimental and Theoretical Investigation and Antibacterial Activity of Synthesized Adducts**” submitted to the Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, for the award of the Degree of **Doctor of Philosophy in Chemistry**, is a record of original research work done by **A.Abinaya**, during the period of her study (**July 2017- March 2023**) in the Department of Chemistry, Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, under my supervision and guidance and the thesis has not formed the basis for the award of any Degree/Diploma/Associateship/Fellowship or similar title to any candidature of any other university.

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DECLARATION

I hereby declare that the thesis entitled “Inverse Electron Demand Diels Alder Reaction of Pyrido[1,2-*a*]pyrimidine-2-ones - Experimental and Theoretical Investigation and Antibacterial Activity of Synthesized Adducts” submitted to the Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, for the award of the **Degree of Doctor of Philosophy in Chemistry**, is a record of original research work done by me under the supervision and guidance of **Dr.V.Sharulatha**, Assistant Professor(SS), Department of Chemistry, Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore and that it has not formed the basis for the award of any Degree/Diploma/Associateship/Fellowship or similar title to any candidature of any University.

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“Thankfulness is the beginning of gratitude. Gratitude is the completion of thankfulness”

– Henri Frederic Amiel

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Abbreviation

DA	Diels-Alder
IEDDAR	Inverse Electron Demand Diels-Alder Reaction
FMOs	Frontier Molecular Orbitals
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
EDG	Electron Donating Group
EWG	Electron Withdrawing Group
SPAAC	Strain-Promoted Azide-Alkyne Cycloaddition
HSA	Human Serum Albumin
LA	Lewis Acid
DK	Diketone
TMS	Trimethyl silane
TLC	Thin layer chromatography
DMF	Dimethylformamide
IP	Ionization Potential
EA	Electron Affinity
SPECT-CT	Single Photo Emission Computed Tomography/ Computed Tomography
AIDS	Acquired Immuno Deficiency Syndrome
MDR	Major Depressive Disorder
FTIR	Fourier Transform Infrared Spectroscopy
¹ H NMR	Proton-Nuclear Magnetic Resonance Spectroscopy
¹³ C NMR	Carbon 13-Nuclear Magnetic Resonance Spectroscopy
ESI-MS	Electrospray Ionization Mass Spectroscopy
PDB	Protein Data Bank
DMSO	Dimethyl sulfoxide
DFT	Density Functional Theory
IEFPCM	Integral Equation Formalism Polarizable Continuum Model
CFU	Colony Forming Unit
RCSB	Research Collaboratory for Structural Bioinformatics

DHFR	Dihydrofolate reductase
THF	Tetrahydrofuran
NADPH	Nicotinamide Adenine Dinucleotide Phosphate
RNA	Ribo Nucleic Acid
DNA	Deoxyribose nucleic acid
UNAM	Uridine diphosphate N acetyl muramic acid
MGL	Molecular Graphics Laboratory
PDBQT	Protein Data Bank, Partial Charge (Q), & Atom Type (T)
ADMET	Absorption Distribution metabolism excretion Toxicity
MW	Molecular Weight
RB	Rotatable Bonds
MR	Molar Refractivity
HBD	Hydrogen Bond Donor
HBA	Hydrogen Bond Acceptor
TPSA	Topological Polar Surface Area
BBB	Blood Brain Barrier
ClogP	Hydrophilicity
Rf	Retention factor
NBO	Natural Bond Orbital
TS	Transition Structure
IRC	Intrinsic Reaction Co-ordinate
K _p	Skin Permeability

Symbols

π	Pi
δ	Delta
μ	Mu
η	Eta
ω	Omega
ΔN_{max}	Maximum electronic charge transfer
σ	Sigma
K _P	Skin permeability
