

CERTIFICATE


I certify that the thesis entitled "**Antirolithiatic Potential of *Spermacoce articularis* L.f. through *In Vivo* and *In Silico* Analysis**" submitted for the award of **Doctor of Philosophy (Ph.D)** by **Gopika S** is the record of research work carried out by her during the period of study under my guidance and supervision, and that this work has not formed the basis for the award of any Degree, Diploma, Associateship, Fellowship or other Titles in this Institute or any other University or Institution of Higher Learning.


26/4/25

**Signature of the
Head of the Department**


26/4/25

Signature of the Supervisor


26/4/2025

Signature of Dean

DECLARATION

I declare that the thesis entitled '**Antiuro lithiatic Potential of *Spermacoce articularis* L.f. through *In Vivo* and *In Silico* Analysis**' submitted by me for the award of **Doctor of Philosophy (Ph.D) by Gopika S** is the record of work carried out by me during the period of study under the guidance of **Dr. M. K. Nisha**, Assistant Professor (SS), Department of Botany, Avinashilingam Institute of Home Science and Higher Education For Women and has not formed the basis for the award of any Degree, Diploma, Associateship, Fellowship, Titles in this Institute or any other University or other similar Institution of Higher Learning.

 26/4/25

Signature of the Supervisor



Signature of the Research Scholar

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LIST OF ABBREVIATIONS

%	-	Percentage
C	-	Degree centigrade
ql	-	Micro litre
pm	-	Micromolar
ABTS	-	2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)
AD	-	Anno Domini
AlCl ₃	-	Aluminium chloride
ANOVA	-	Analysis of Variance
AQ	-	Aqueous
ASP	-	Aspartic acid
BC	-	Before Christ
BHA	-	Butylated hydroxyanisole
BHT	-	Butylated Hydroxy Toluene
BUN	-	Blood Urea Nitrogen
CaC ₂ O ₄	-	Calcium oxalate
CaCl ₂	-	Calcium chloride
CaOx	-	Calcium oxalate
CAT	-	Catalase
CD	-	Critical Difference
CH	-	Chloroform
cm	-	Centimetre
COD	-	Calcium oxalate dehydrate
COM	-	Calcium monohydrate crystals
Conc.	-	Concentration
CYS	-	Cysteine
CYS	-	Cystine
dl	-	Decilitre
DNPH	-	2,4- 2,4-Dinitrophenyl hydrazine reagent
DNTB	-	5'5-dithiobis-2-nitrobenzoic acid
DPPH	-	2, 2-diphenyl-2-picryl hydrazyl hydrate
EDTA	-	Ethylene Diamine Tetra Acetic Acid
EG	-	Ethylene glycol
ESWL	-	Extracorporeal Shock Wave Lithotripsy
Fe	-	Iron
Fe ₂	-	Ferrous ion
Fe ₃	-	Ferric ion
FeCl ₃	-	Ferric chloride
FT-IR	-	Fourier Transform - Infrared Spectroscopy

<i>G</i>	-	<i>Gram</i>
<i>GC-MS</i>	-	<i>Gas chromatography- Mass Spectrometry</i>
<i>GLY</i>	-	<i>Glycine</i>
<i>GSH</i>	-	<i>Reduced Glutathione</i>
<i>h</i>	-	<i>Hour</i>
<i>H₂O₂</i>	-	<i>Hydrogen peroxide</i>
<i>H₂SO₄</i>	-	<i>Sulphuric acid</i>
<i>HCl</i>	-	<i>Hydrochloric acid</i>
<i>HNO₃</i>	-	<i>Nitric oxide</i>
<i>HPTLC</i>	-	<i>High Performance Thin Layer Chromatography</i>
<i>IAEC</i>	-	<i>Institutional Animal Ethics Committee</i>
<i>IC</i>	-	<i>Inhibition Concentration</i>
<i>Ir</i>	-	<i>Inhibition rate</i>
<i>IR</i>	-	<i>Infra Red</i>
<i>LD</i>	-	<i>Lethal Dose</i>
<i>LigPrep</i>	-	<i>Ligand preparation</i>
<i>M</i>	-	<i>Molar</i>
<i>m/e</i>	-	<i>Mass by charge</i>
<i>Me</i>	-	<i>Methanol</i>
<i>mg</i>	-	<i>Milligram</i>
<i>min</i>	-	<i>Minute</i>
<i>ml</i>	-	<i>Millilitre</i>
<i>mM</i>	-	<i>Millimolar</i>
<i>N</i>	-	<i>Normality</i>
<i>Na₂C₂O₄</i>	-	<i>Sodium oxalate</i>
<i>NaCl</i>	-	<i>Sodium chloride</i>
<i>NaNO₂</i>	-	<i>Sodium nitrite</i>
<i>NaOH</i>	-	<i>Sodium hydroxide</i>
<i>NIST</i>	-	<i>National Institute of Standards and Technology</i>
<i>Nm</i>	-	<i>Nanometer</i>
<i>Nmoles</i>	-	<i>Nanomoles</i>
<i>NO</i>	-	<i>Nitric oxide</i>
<i>OD</i>	-	<i>Optical density</i>
<i>PB</i>	-	<i>Phosphate Buffer</i>
<i>PDB</i>	-	<i>Protein Data Bank</i>
<i>PE</i>	-	<i>Petroleum ether</i>
<i>PHE</i>	-	<i>Phenylalanine</i>
<i>PPO</i>	-	<i>Polyphenol Oxidase</i>
<i>ROS</i>	-	<i>Reactive Oxygen Species</i>
<i>Rpm</i>	-	<i>Revolutions per minute</i>
<i>RT</i>	-	<i>Retention Time</i>
<i>SD</i>	-	<i>Standard Deviation</i>
<i>SE</i>	-	<i>Standard Error</i>

SED	-	Standard Error Deviation
SER	-	Serine
SOD	-	Superoxide dismutase
TLC	-	Thin layer chromatography
TCA	-	Trichloro acetic acid
THP	-	Tamm-Horsfall protein
THR	-	Threonine
TYR	-	Tyrosine
PG	-	Propyl Gallate
UV	-	Ultra Violet
Ver	-	Version
A	-	Alpha
B	-	Beta
MDS	-	Molecular dynamics simulation
RMSD	-	The root-mean-square-deviation
RMSF	-	Root-mean-square-fluctuation
ROG	-	radius of gyration
LVR5	-	Lipinski's violation rule of five
ADMET	-	Absorption, Distribution, Metabolism, Excretion, and Toxicity
DMPK	-	Drug Metabolism and Pharmacokinetics
BBB	-	Blood-brain barrier
PPB	-	Plasma protein binding
nHBAs	-	Number of hydrogen bond acceptors
nHBDs	-	Number of hydrogen bonds
PSA	-	Polar Surface Area
P-gp	-	p – glycoprotein
CYP1A	-	Cytochrome P450 Enzyme Subfamily
rGYr	-	Radius of gyration
PSA	-	Polar surface area
Intra HB	-	Intramolecular hydrogen bonding
MolSA	-	Molecular surface area
SASA	-	Solvent accessible surface area
UMOD	-	Uromodulin
PDB	-	Protein Data Bank
DS	-	Docking score
Å	-	Angstrom
n sec	-	Nanoseconds
Glide	-	Grid-based Ligand Docking with Energetics
RCSB	-	Research Collaboratory for Structural Bioinformatics
SMILES	-	Simplified molecular input line entry specification
XP	-	Xtra Precision
2D	-	2-Dimensional
3D	-	3-Dimensional
