CERTIFICATE

I certify that the thesis entitled "**Antiurolithiatic 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 '**Antiurolithiatic 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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Gopika Sreenivasan

LIST OF TABLES

LIST OF FIGURES

LIST OF PLATES

LIST OF APPENDICES

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_2O_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*

G	-	*Gram*
GC-MS	-	*Gas chromatography- Mass Spectrometry*
GLY	-	*Glycine*
GSH	-	*Reduced Glutathione*
h	-	*Hour*
H_2O_2	-	*Hydrogen peroxide*
H_2SO_4	-	*Sulphuric acid*
HCl	-	*Hydrochloric acid*
HNO_3	-	*Nitric oxide*
HPTLC	-	*High Performance Thin Layer Chromatography*
IAEC	-	*Institutional Animal Ethics Committee*
IC	-	*Inhibition Concentration*
Ir	-	*Inhibition rate*
IR	-	*Infra Red*
LD	-	*Lethal Dose*
LigPrep	-	*Ligand preparation*
M	-	*Molar*
m/e	-	*Mass by charge*
Me	-	*Methanol*
mg	-	*Milligram*
min	-	*Minute*
ml	-	*Millilitre*
mM	-	*Millimolar*
N	-	*Normality*
$Na_2C_2O_4$	-	*Sodium oxalate*
NaCl	-	*Sodium chloride*
$NaNO_2$	-	*Sodium nitrite*
NaOH	-	*Sodium hydroxide*
NIST	-	*National Institute of Standards and Technology*
Nm	-	*Nanometer*
Nmoles	-	*Nanomoles*
NO	-	*Nitric oxide*
OD	-	*Optical density*
PB	-	*Phosphate Buffer*
PDB	-	*Protein Data Bank*
PE	-	*Petroleum ether*
PHE	-	*Phenylalanine*
PPO	-	*Polyphenol Oxidase*
ROS	-	*Reactive Oxygen Species*
Rpm	-	*Revolutions per minute*
RT	-	*Retention Time*
SD	-	*Standard Deviation*
SE	-	*Standard Error*

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*