

## TABLE OF CONTENTS

List of Figures	I
List of Tables	V
Abbreviations	VI
Preface	VIII
1 Introduction	1
2 Literature review	6
2.1 Plant description	6
2.1.1 Taxonomy	8
2.1.2 Distribution	8
2.2 Reported phytoconstituents and ethnopharmacology	9
2.3 Network Pharmacology	11
2.4 Pharmacological studies	13
2.4.1 Antibacterial activity	13
2.4.2 Anti-inflammatory activity	14
3 Rationale, objectives, and plan of work	16
3.1 Rationale	16
3.2 Objectives	17
3.3 Plan of work	18
4 Material and methods	19
4.1 Collection and identification of plant material	19
4.2 DNA Barcoding	19
4.2.1 Extraction of DNA	19
4.2.2 PCR Amplification	20
4.2.3 DNA Sequencing and analysis	21
4.3 Quality control assessment	22

4.3.1	Morphological and microscopical study	22
4.3.2	Physicochemical analyses	22
4.3.3	Loss on drying	23
4.3.4	Ash value	23
4.3.5	Extractive value	24
4.3.6	Foaming index	24
4.3.7	Heavy metals and aflatoxins analyses	25
4.4	Preparation of plant extract	25
4.5	Animal selection and care	26
4.6	Acute toxicity study	26
4.7	Repeated dose 28-day oral toxicity study	27
4.8	Qualitative analysis using LC-MS	27
4.9	Network Pharmacology-based prediction	28
4.9.1	Compound target prediction and in-silico drug-likeness screening	28
4.9.2	Antibacterial potential prediction	28
4.9.3	Anti-inflammatory potential prediction	29
4.10	In vitro antibacterial study	30
4.10.1	Microbial strains and culture media	30
4.10.2	Sample preparation	31
4.10.3	Agar well diffusion method	31
4.10.4	Microtiter-plate dilution method	31
4.11	Molecular Docking studies and MM-GBSA studies	32
4.11.1	Ligand selection and preparation	32
4.11.2	Protein selection and preparation	33
4.11.3	Grid generation	33
4.11.4	Molecular docking	33

4.12	Molecular Dynamic simulation study	34
4.13	In vitro anti-inflammatory assays	34
4.13.1	Protein denaturation method	34
4.13.2	Proteinase inhibition	35
4.13.3	Membrane stability	35
4.14	Carrageenan-induced paw oedema method	36
4.15	Statistical analysis	37
5	Results	38
5.1	DNA barcoding	38
5.2	Quality control assessment	38
5.3	Acute toxicity study	43
5.4	Repeated dose 28-day oral toxicity study	43
5.5	Qualitative analysis using LC-MS	48
5.6	Network Pharmacology Prediction	54
5.6.1	Antibacterial potential	54
5.6.2	Anti-inflammatory potential	57
5.7	In vitro antibacterial activity	63
5.8	Molecular Docking studies	64
5.9	Molecular Dynamic simulation study	71
5.10	In vitro anti-inflammatory activity	73
5.11	In vivo anti-inflammatory activity	74
6	Discussion	76
7	Summary and conclusion	83
	References	84
	Appendix I	i
	List of Publications	xxx