

**SUBMISSION FOR EVALUATION
FINAL YEAR PROJECT 2 - RESEARCH PROJECT**

**INVESTIGATING PHYTOTOXICITY REMOVAL OF CHLOROGENIC
ACID (CGA) AND CAFFEINE FROM SPENT COFFEE GROUND (SCG)
USING CHEMICAL AND THERMAL PRETREATMENT**

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TABLE OF CONTENT

ACKNOWLEDGEMENTS	I
LIST OF TABLES	V
LIST OF FIGURES	VII
LIST OF SYMBOLS	IX
LIST OF ABBREVIATIONS	X
ABSTRACT	XI
ABSTRAK	XII
CHAPTER 1 INRODUCTION	1
1.1 Back ground of study	1
1.2 Problem statement	3
1.3 Objectives of study	4
1.4 Significance of study	4
1.5 Expected Output/Outcomes/Implication	6
CHAPTER 2 LITERATURE REVIEW	7
2.1 Spent coffee ground (SCG)	7
2.2 Phytotoxic compounds in SCG	8
2.2.1 Chlorogenic acid	10
2.2.2 Caffeine	10
2.3 SCG as soil amendment	12
2.4 Pre-treatment of SCG	13
2.4.1 Conventional extraction (CSE)	14
2.4.2 Ultra-sound assisted extraction (UAE)	15
2.4.3 Microwave assisted extraction (MAE)	16
2.4.4 Supercritical fluid (SFE)	17
2.4.5 Carbonisation of SCG	19
2.5 Design of Experiment	20

METHODOLOGY	21
3.1 Materials	21
3.2 Chemicals	21
3.3 Apparatus and equipment	21
3.4 Instrument	21
3.5 Chemical Pretreatment of SCG	22
3.5.1 RSM for chemical pretreatment	22
3.6 Thermal Pretreatment of SCG	24
3.6.1 RSM for thermal pretreatment	24
3.7 UV-Vis analysis	25
3.8 HPLC analysis	26
3.9 Characterisation of Untreated and Treated SCG	26
3.9.1 FTIR spectra analysis	27
3.9.2 ICP-OES Analysis	27
3.10 Experimental design/flow chart	28
CHAPTER 4 RESULTS AND DISCUSSION	29
4.1 Optimization of Phytotoxicity Removal from Spent Coffee Grounds via Chemical Pre-treatment Using Response Surface Methodology.	29
4.1.1 Yield of SCG After Chemical pre-treatment.	30
4.1.2 Parametric Study of SCG Yield by Chemical Pre-treatment	31
4.1.3 Caffeine Removal.	33
4.1.4 Parametric Study of Caffeine Removal by Chemical Pre-treatment	34
4.1.5 CGA Removal by Chemical Pre-treatment	36
4.1.6 Parametric Study of CGA Removal by Chemical Pre-treatment	39
4.1.7 Optimization and Validation Experiment for Chemical Pretreatment	41
4.2 Optimization of Phytotoxicity Removal from Spent Coffee Grounds via Thermal Pre-treatment Using Response Surface Methodology.	42
4.2.1 Yield of SCG after thermal pre-treatment.	42
4.2.3 Caffeine Removal by Thermal Pre-treatment.	46
4.2.4 Parametric Study of Caffeine Removal by Thermal Pre-treatment	48
4.2.5 Evaluation of Residual Chlorogenic Acid in Spent Coffee Grounds after Thermal Pre-treatment Using Response Surface Methodology	50
4.2.6 Parametric Study of CGA Removal by Thermal Pre-treatment	51

ABSTRACT

INVESTIGATING PHYTOTOXICITY REMOVAL OF CHLOROGENIC ACID (CGA) AND CAFFEINE FROM SCG USING CHEMICAL AND THERMAL PRETREATMENT

Spent coffee grounds (SCG), a by-product of the global coffee industry, contain valuable organic matter and nutrients but are limited in agricultural applications due to the presence of phytotoxic compounds such as chlorogenic acid (CGA) and caffeine. These compounds can suppress plant growth and microbial activity in soil. This study investigates the removal of CGA and caffeine from SCG using two pretreatment methods: chemical (ultrasound-assisted extraction) and thermal (carbonisation), with the goal of reducing phytotoxicity and enabling safe reuse as soil amendments. Response Surface Methodology (RSM) was applied to optimise treatment parameters, particularly temperature and reaction time. The optimum condition for chemical pretreatment of spent coffee grounds was 80 °C for 10 min, while thermal pretreatment was optimized at 400 °C for 120 min. Following treatment, SCG samples were analysed using Fourier-transform infrared spectroscopy (FTIR), high-performance liquid chromatography (HPLC), ultraviolet-visible spectroscopy (UV-Vis), and inductively coupled plasma optical emission spectrometry (ICP-OES) to evaluate chemical composition, phytotoxic compound removal, and nutrient content. FTIR results for both chemical and thermal pretreatment indicated significant reductions in peaks at 1700 cm^{-1} (C=O) and 3200–3400 cm^{-1} (O–H), suggesting degradation of phytotoxic substances. Weaker aliphatic C–H signals (2850–2920 cm^{-1}) indicated partial caffeine removal. HPLC and UV-Vis confirmed reductions in CGA and caffeine, correlating with increased treatment severity. Elemental analysis of untreated SCG showed the presence of K (0.41 mg/g), Zn (0.26 mg/g), Cu (0.08 mg/g), and Fe (16.83 mg/g). Chemical treatment decreased metal content, while thermal treatment increased nutrients' concentrations due to organic matter loss, particularly enriching iron. The findings demonstrate that both pretreatment methods effectively reduce phytotoxicity in SCG. This supports the development of an affordable, sustainable detoxification process for SCG valorisation in agriculture.