Table of Contents

Abstract			i
Declaration			ii
Certificate			iii
Acknowledgements			iv-v
Contents			vi-xiii
List of tables			xiv-xv
List of figures			xvi-xxi
List of abbreviations			xxii-xxiv
Chapter 1 Introduction			
1.1	Introduction		
	1.2.1	Classification of peaches	2, 3
	1.2.2	Geographical Distribution of peaches	3
	1.3.1	Dietary Phytochemicals	3,4
	1.3.2	Therapeutic effects of phytochemicals	4,5
	1.3.3	Peach Phytochemicals	5,6
	1.3.4	Therapeutic Effects of Peach	6,7
	1.3.5	Anti-inflammatory activity	8
	1.3.6	Anticancer activity	8,9
1.4	Analytical Methods		
	1.4.1	Phytochemical Extraction Methods	9,10
	1.4.2	Separation and quantification methods	10,11
	1.4.3	Computer-aided drug designing	11
	1.4.4	Encapsulation of phytochemicals	11,12
	1.4.5	Incorporation of phytochemicals in a food product	12
1.5	Hypothesis		13
1.6	Gap of research		13
1.7	Objectives		14
	References		14-20
Chapter 2 To extract bioactive compounds from fruits of Norabogori (*Prunus persica* L. Batsch) and their quantification and characterization			
2.1	Introduction		22-24
2.2	Materials and methods		
	2.2.1	Chemicals	24
	2.2.2	Plant sample collection and preparation	24

	2.2.3	Chemical composition		25
	2.2.4	Extraction of phytochemicals		25
		2.2.4.1	Conventional extraction of phytochemicals	25
		2.2.4.2	Total phenolic content (TPC)	25
		2.2.4.3	Microwave-assisted extraction of phytochemicals	25-26
			2.2.4.3.1 Optimization using Box-Behnken design (BBD)	26-27
			2.2.4.3.2 Optimization and validation	28
	2.2.5	Identification of major compounds in the norabogori extract by Hr-LCMS		28
	2.2.6	Phytochemicals analysis using Reverse-Phase High-Performance Liquid Chromatography (RP-HPLC)		28-29
	2.2.7	Statistical analysis		29
2.3	Results and discussion			
	2.3.1	Specimen identification		29
	2.3.2	Chemical compositionof norabogori fruit		30
	2.3.3	Conventional extraction of phytochemicals		31-32
		2.3.4.1	Optimization and fitting of the model	32-33
		2.3.4.2	Microwave-assisted extraction performance	33-35
		2.3.4.3	Validation of the optimized conditions	35
		2.3.4.4	Verification of the predictive model	35-36
	2.3.5	Identification of major compounds in the norabogori extract by Hr-LCMS		36-38
	2.3.6	Phytochemical analysis of norabogori fruit extract using RP-HPLC		38-40
	2.3.7	Conclusion		40-41
		References		41-43
Chapter 3 To study the in vitro anti-oxidant, anti-inflammatory and anti-cancer activity of the norabogori extract				
3.1	Introduction			45-47
3.2	Materials and methods			
	3.2.1	Chemicals and reagents		47
	3.2.2	Sample preparation		47
	3.2.3	Purification of Norabogori extract		47
	3.2.4	Antioxidant activity		
		3.2.4.1	DPPH free radical scavenging activity	47-48
		3.2.4.2	ABTS Radical Cation Decolorization Assay	48
		3.2.4.3	IC_{50} Value Calculation	48
	3.2.5	Cell line and culture		49

	3.2.6	Cytotoxicity assay	49
	3.2.7	Effect of Norabogori extract on pro-inflammatory marker	
		3.2.7.1 Cell Treatments	49
		3.2.7.2 Isolation of total RNA and RT-PCR	50
	3.2.8	Anti-cancer activity of Norabogori extract by MTT assay	50
	3.2.9	Statistical Analysis	50
3.3	Results		
	3.3.1	Antioxidant activity of norabogori fruit extract	
		3.3.1.1 DPPH free radical scavenging activity	51-52
		3.3.1.2 ABTS Scavenging Activity	52-53
	3.3.2	Norabogori extract regulates expression of proinflammatory genes	
		3.3.2.1 Cell viability assay	53-54
		3.3.2.2 Effect of norabogori extract on pro-inflammatory genes	54-55
	3.3.3	Anti-cancer activity of Norabogori extract by MTT assay	56-57
3.4	Conclusion		58
	References		58-61

Chapter 4 To study the in silico anti-inflammatory activity of the norabogori extract

4.1	Introduction		63-67
4.2	Materials And Methods		
	4.2.1	Phytochemical database preparation	68
	4.2.2	Evaluation of phytochemicals	68
	4.2.3	Ligand structure retrieval	69
	4.2.4	Ligand structure preparation	69
	4.2.5	Protein structure retrieval	69
	4.2.6	Protein structure preparation	69
	4.2.7	Sequence alignment and homology modeling	69-70
	4.2.8	Molecular docking studies	70
	4.2.9	Molecular dynamics simulation	71-72
4.3	Results and discussion		
	4.3.1	Lipinski’s Rule of Five and Veber's rule evaluation	72-74
	4.3.2	ADMET properties evaluation	74-79
	4.3.3	Protein Structural retrieval	79-83
	4.3.4	Sequence allignment and homology modelling	83
	4.3.5	Molecular docking studies	83-87
	4.3.6	Molecular dynamics simulation	88-96
4.4	Conclusion		97
	References		97-100

Chapter 5 To develop functional food product by incorporating encapsulated Norabogori extract

5.1 Introduction 102-104

5.2 Materials and methods 104

5.2.1 Sample preparation 104

5.2.2 Development of norabogori leather 104-105

5.2.2.1 Color analysis of norabogori fruit leather 105

5.2.2.2 Textural properties of norabogori fruit leather 105-106

5.2.3 Microencapsulation of crude extract 106

5.2.4 Physicochemical characterizations of microbeads

5.2.4.1 Encapsulation efficiency 106-107

5.2.4.2 In vitro simulated gastro-intestinal digestion release study of the micro-encapsulates 107

5.2.4.3 Microparticle size analysis by Scanning Electron Microscope (SEM) 107

5.2.4.4 DPPH assay 107-108

5.2.5 Fortification of microencapsulate to norabogori leather

5.2.5.1 Fruit leather development 108

5.2.5.2 Physico-chemical characteristics of norabogori fruit leather 108

5.2.5.3 Sensory acceptability analysis of norabogori leather with encapsulate 108

5.2.6 Statistical analysis 109

5.3 Results and Discussion

5.3.1 Development of norabogori leather 109

5.3.1.1 Color analysis 109

5.3.1.2 Textural properties 110

5.3.2 Encapsulation of the norabogori extract analysis

5.3.2.1 Encapulation efficiency 111-112

5.3.2.2 In vitro gastrointestinal release of the microencapsulate under simulated conditions 112-113

		5.3.2.3	Microparticle morphology analysis by Scanning Electron Microscope (SEM)	113
	5.3.3	Encapsulate incorporated leather development		
		5.3.3.1	Texture analysis of encapsulate incorporated leather	114
		5.3.3.2	Physico-chemical characteristics of norabogori fruit leather	114-115
		5.3.3.3	Sensory evaluation of the final product	115
5.4	Conclusion			116
	References			116-119

Chapter 6 Conclusions and future scope of work

6.1	Conclusions		121-122
6.2	Future scope of the present investigation		122
6.3	Research publications		123
	6.3.1	Journal publications	123
	6.3.2	Under-process / to be communicated	123
6.4	Training/ workshop attended		123