

Candidate's Declaration

I hereby declare that the thesis entitled “**Assessment of Phyto-pharmaceutical compounds present in the food-based medicinal formulation of macerated garlic (*Allium sativum* L) in boiled mustard (*Brassica nigra* L.) oil**” has been submitted to the **Department of Molecular Biology and Biotechnology, Tezpur University, Tezpur, Assam** in partial fulfilment for the award of degree of Doctor of Philosophy in Molecular Biology and Biotechnology is an original work undertaken by me. Further, I declare that no part of the work has been previously considered for the award of any other degree from any University, Institute, or other organization.

Date: 29/4/2025

Place: Tezpur



Joydeep Singha

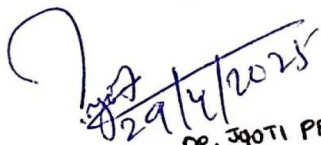


TEZPUR UNIVERSITY
(A Central University established by an Act of Parliament)
Department of Molecular Biology and Biotechnology
NAPAAM, TEZPUR-784028, ASSAM, INDIA

CERTIFICATE OF THE SUPERVISORS

This is to certify that the thesis entitled “**Assessment of Phyto-pharmaceutical compounds present in the food-based medicinal formulation of macerated garlic (*Allium sativum* L) in boiled mustard (*Brassica nigra* L.) oil**” submitted to the School of Sciences, Tezpur University in part fulfilment for the award of the degree of Doctor of Philosophy in Department of Molecular Biology and Biotechnology, is a record of original research work carried out by Mr. Joydeep Singha under my supervision and guidance.

All help received by him from various sources has been duly acknowledged. No part of the thesis has been reproduced elsewhere for the award of any other degree.


29/4/2025

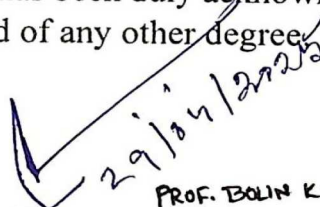
DR. JYOTI PRASAD SRIKIA

Signature of Supervisor

Designation: Assistant Professor

School: Sciences

Department: Molecular Biology
and Biotechnology


29/4/2025

PROF. BOLIN KUMAR KONWAR

Signature of Co-Supervisor

Designation: Professor

Affiliation: Department of Molecular
Biology and Biotechnology, Tezpur
University, Tezpur.

Candidate's Declaration

I hereby declare that the thesis entitled “**Assessment of Phyto-pharmaceutical compounds present in the food-based medicinal formulation of macerated garlic (*Allium sativum* L.) in boiled mustard (*Brassica nigra* L.) oil**” has been submitted to the **Department of Molecular Biology and Biotechnology, Tezpur University**, Tezpur, Assam in partial fulfilment for the award of degree of Doctor of Philosophy in Molecular Biology and Biotechnology is an original work undertaken by me. Further, I declare that no part of the work has been previously considered for the award of any other degree from any University, Institute, or other organization.

Date:

Joydeep Singha

Place: Tezpur



TEZPUR UNIVERSITY
(A Central University established by an Act of Parliament)
Department of Molecular Biology and Biotechnology
NAPAAM, TEZPUR-784028, ASSAM, INDIA

CERTIFICATE OF THE SUPERVISORS

This is to certify that the thesis entitled “**Assessment of Phyto-pharmaceutical compounds present in the food-based medicinal formulation of macerated garlic (*Allium sativum* L) in boiled mustard (*Brassica nigra* L.) oil**” submitted to the School of Sciences, Tezpur University in part fulfilment for the award of the degree of Doctor of Philosophy in Department of Molecular Biology and Biotechnology, is a record of original research work carried out by Mr. Joydeep Singha under my supervision and guidance.

All help received by him from various sources has been duly acknowledged. No part of the thesis has been reproduced elsewhere for the award of any other degree.

Signature of Supervisor

Designation: Assistant Professor

School: Sciences

Department: Molecular Biology
and Biotechnology

Signature of Co-Supervisor

Designation: Professor

Affiliation: Department of Molecular
Biology and Biotechnology, Tezpur
University, Tezpur.

Acknowledgement

First and foremost, I express sincere gratitude to my supervisor, Dr. Jyoti Prasad Saikia, for trusting me and for allowing me to pursue my doctoral research under his supervision. I thank him for his guidance, encouragement and patience throughout my Ph.D. There is so much that I have learned from him during this journey that I can never thank him enough.

I would also like to thank my Co-supervisor, Professor Bolin Kumar Konwar, for his support and encouragement during my PhD journey.

I take this opportunity to acknowledge Tezpur University, the University Grants Commission, Govt. of India and the Department of Biotechnology (DBT) for providing me with a fellowship during my Ph.D. tenure.

I thank the Hon'ble Vice Chancellors, Professor Shambhu Nath Singh of Tezpur University for providing all the necessary facilities for education and research on the campus. I thank the entire Tezpur University fraternity for their help and support. I thank Saraighat CV Raman Men's Hostel for being my home away from home. I extend my heartfelt gratitude to the Department of Molecular Biology and Biotechnology for providing all the necessary facilities for research along with the ambience of a family. I thank all the faculty members of the department for extending their laboratory facilities. I sincerely thank my doctoral committee members, Prof. Suvendra Kumar Ray, Prof. Manabendra Mandal and Dr. Pankaj Barah, for their valuable suggestions and recommendations. I also thank all the technical and non-technical staff of the department of MBBT for their help and support.

I would like to thank Prof. Manabendra Mandal for providing the bacterial and fungal strains for carrying out my research work. I would also like to thank Dr. Rupak Mukhopadhyay for allowing me to carry out the cell culture work in his laboratory.

I express my sincere gratitude to our current and previous heads of the department for allowing me to use all the facilities and addressing any issues raised.

I would like to thank the SAIC facilities of Tezpur University for providing us with instruments used in carrying out the experiments; special thanks to Mr Sankur, Mr Boro, Mr Prakash Kurmi and Dr Nipu Dutta. I am thankful to the University Library for its facilities, with special mention to Mr Jitu Mani Das for his quick response to plagiarism checks and queries.

I thank my lab mates Dr Minhaz Ahmed, Santanu Goswami, Monalisha Chutia and Isheeta Singha for creating and maintaining a healthy research environment in the lab. I thank all the project students who have worked with me and helped me learn during the process. I thank all my seniors and juniors from the department of MBBT for their help and friendship. I thank M.Sc. and Int. M.Sc. project students Kipjyoti, Azhar, Santanu, Sunita, Romit, Janefa, Sanjibani, Bahnishikha, Bishakha, Moumita, Richa, Sohum, Isheeta.

I would like to thank Dr Jharna Choudhury for her constant support, both emotionally and financially during my PhD journey. I will always be grateful for your all love, care and support.

I would like to thank Anupam Dutta, Rituraj Chakraborty and Santanu Goswami for working as a collaborator. I would like to thank my juniors Bahnishikha Roy, Vishakha

Biswakarma, Moumita Jana and Isheeta Singha for helping me during my research work. I would like to thank Shubham for helping me during my experimental work. I would like to thank Miss Rubismita Deka for helping me during carrying out the experiments and during the preparation of the diffusion cell.

Most importantly, I would like to express my deepest gratitude to my parents (Mr Jitendra Singha and Mrs Dipti Singha), my elder sister (Dr Jasmine Singha) and my younger sister (Sanjana Singha) for the emotional and financial support. I also would like to thank my grandmother (Late Molika Singha) for always loving me unconditionally. Thank you for being there.

Date:

(Joydeep Singha)

Place: Tezpur

LISTS OF FIGURES

Figure No.	Title	Page No.
1	Flowchart of the chemical breakdown of allicin in non-polar solvents and vegetable oils.	19
2	(A) Liquid chromatogram of GMM, (B) mass spectrometric data at retention time between 2.67 and 3.24 minutes.	40
3	(A) Prepared eggshell membrane; (B) diffusion cell prepared in laboratory.	55
4	Free fatty acid content in MO and GMM. Note: NS- Not significant.	62
5	Peroxide value of MO, HMO, and GMM. Note: NS- Not significant, *- at $p < 0.05$, ** - at $p < 0.01$.	63
6	Acid value of GMM and MO. Note: NS- Not significant	63
7	Iodine value of MO and GMM. Note: NS- Not significant.	64
8	Saponification value of mustard oil, and garlic mustard oil macerate. Note: NS- Not significant.	64
9	(A) FTIR spectroscopy of MO, HMO, GMM1 and GMM2 from 400-4000 cm^{-1} ; (B) FTIR spectroscopy of MO, HMO, GMM1 and GMM2 from 2500-3200 cm^{-1}	66
10	Total polyphenolic content in MO and GMM. Note: ** - at $p < 0.01$.	67
11	DPPH scavenging activity of lipophilic and hydrophilic parts of GMM and MO. NS- Non significant, *** at $p < 0.001$.	68
12	Thin layer chromatography analysis of MO, GMM and raw garlic.	69
13	HPLC chromatogram of mustard oil (MO), garlic mustard oil macerate (GMM), and garlic toluene extract (GTE).	69
14	(A) Liquid chromatogram during LC/MS analysis of GTE; mass spectrometry data at retention time (B) 0.826 min (C) 0.978 min.	70
15	Mass spectrometry data of GTE at retention time (A) 2.346 min; (B) 1.260 min and (C) 1.933 min.	71
16	(A) Liquid chromatogram during LC/MS analysis of MO; mass spectrometry data at retention time (B) 0.804 min (C) 1.130 min.	72
17	Mass spectrometry data of MO at retention time (A) 1.26; (B) 1.50; (C) 5.34; and (D) 7.17 min.	73
18	Mass spectrometry data of MO at retention time 8.45 min.	74
19	(A) Liquid chromatogram during LC/MS analysis of GMM; mass spectrometry data at retention time (B) 0.82 min.	74
20	(A) Mass spectrometry data of GMM at retention time 0.85; (B) zoomed image of the region of 163.00 m/z at retention time 0.85 min; and (C) mass spectrometry data of GMM at retention time 0.98 min.	75
21	(A) Mass spectrometry data of GMM at retention time 1.09; (B) 1.48 min; and (C) 3.00 min.	76
22	(A) Mass spectrometry data of GMM at retention time 5.34; (B) retention time 7.14 min; and (C) 9.14 min.	77
23	Shows a response surface plot for optimization of ajoene for (A) temperature and time, (B) time and amount of oil, and (C) temperature and amount of oil for GMM preparation; and a response surface plot for 2-vinyl-4H-1,3, dithiin optimization with (D) temperature, (E) time, and (F) amount of oil for GMM preparation.	83

24	Showing the antibacterial activity against <i>S. aureus</i> MTCC 3160 when exposed to different volumes of mustard oil and garlic mustard oil macerate vapour.	84
25	Showing the antibacterial activity against <i>K. pneumoniae</i> MTCC 618 when exposed to different volumes of mustard oil and garlic mustard oil macerate vapour.	84
26	Showing the antibacterial activity against <i>E. coli</i> MTCC 40 when exposed to different volumes of mustard oil and garlic mustard oil macerate vapour.	85
27	Showing the antifungal activity against <i>C. albicans</i> MTCC 183 when exposed to different volumes of mustard oil and garlic mustard oil macerate vapour.	86
28	Antibacterial activity against <i>S. aureus</i> by prepared GMM at various ratios of garlic and mustard oil by vapour diffusion method.	87
29	Antibacterial activity against <i>S. aureus</i> by prepared GMM sample based on time of heating through vapour diffusion method.	88
30	Antifungal activity of GMM prepared at different temperatures against <i>C. albicans</i> .	88
31	Line graph showing antifungal activity of GMM prepared at different temperatures against <i>C. albicans</i> through agar diffusion method.	89
32	Antifungal activity of GMM heated for different times against <i>C. albicans</i> through agar diffusion method.	89
33	Line graph showing antifungal activity of GMM heated for different times against <i>C. albicans</i> through agar diffusion method.	90
34	Antifungal activity of GMM prepared with different ratios of garlic and mustard oil against <i>C. albicans</i> through agar diffusion method.	90
35	Line graph showing antifungal activity of GMM prepared with different ratios of garlic and mustard oil against <i>C. albicans</i> through agar diffusion method.	91
36	Antifungal activity against <i>C. albicans</i> MTCC 183 by prepared GMM sample with different ratios of garlic and mustard oil through vapour diffusion method after 96 hours of incubation.	92
37	Antifungal activity against <i>C. albicans</i> by prepared GMM heated for different times at 160°C through vapour diffusion method.	93
38	Antifungal activity against <i>Candida albicans</i> MTCC 183 by prepared GMM heated for different times at 80°C through vapour diffusion method.	94
39	DPPH scavenging activity by preparing GMM with different ratios of garlic and mustard oil.	95
40	DPPH scavenging activity by prepared GMM with different temperatures of heating.	95
41	DPPH scavenging activity by preparing GMM with different times for heating.	96
42	Vapour diffusion assay against <i>S. aureus</i> after treatment of MO and GMM vapour.	96
43	Vapour diffusion assay against <i>B. cereus</i> after treatment of MO and GMM vapour.	97
44	Vapour diffusion assay against <i>K. pneumoniae</i> after treatment of MO and GMM vapour.	97
45	Vapour diffusion assay against <i>E. coli</i> after treatment of MO and GMM vapour.	98

46	Minimum inhibitory concentration determination against <i>S. aureus</i> , <i>B. cereus</i> , <i>K. pneumoniae</i> and <i>E. coli</i> by various dilutions of optimized garlic mustard oil macerate. 1=MO, 2=GMM, 3=GMM/2, 4=GMM/4, 5=GMM/8, 6=GMM/16.	98
47	Zone of inhibition during the minimum inhibitory concentration determination against <i>S. aureus</i> , <i>B. cereus</i> , <i>K. pneumoniae</i> and <i>E. coli</i> by various dilutions of optimized garlic mustard oil macerate. N.D.- Not detected.	99
48	Gram staining of different bacterial species after agar diffusion with MO and GMM.	100
49	Showing the increase in zone of inhibition by Gentamycin (G) (10 ng), Tetracycline (T) (10 ng) and kanamycin (K) (10 ng) against <i>S. aureus</i> MTCC 3160 when treated with vapour of mustard oil and garlic mustard oil macerate.	101
50	Representation of the increase in zone of inhibition when <i>S. aureus</i> when exposed to VOCs of MO and GMM.	101
51	(A) FTIR analysis of the staphyloxanthin pigment extract from MO and GMM VOCs treated <i>S. aureus</i> cells; (B) FTIR analysis of <i>S. aureus</i> cells treated with VOCs of MO and GMM.	102
52	(A, B, C) SEM image of control, MO and GMM-treated <i>S. aureus</i> cells respectively.	103
53	Representation of 3D and 2D interaction of crtM with AITC.	104
54	Representation of 3D and 2D interaction of crtM with Dithiin.	104
55	Representation of 3D and 2D interaction of crtM with sinigrin.	105
56	Representation of 3D and 2D interaction of crtM with allicin.	105
57	Representation of 3D and 2D interaction of crtM with ajoene.	105
58	(A) Biofilm production by <i>S. aureus</i> ; (B, C, D) no biofilm production by <i>B. cereus</i> , <i>K. pneumoniae</i> and <i>E. coli</i> , respectively.	106
59	GMM inhibited the <i>S. aureus</i> while no antibacterial activity was observed under the MO.	106
60	(A) <i>S. aureus</i> spread on CRA plate forming biofilm without any treatment; (B) <i>S. aureus</i> forming patches of biofilm in CRA after treatment of MO vapour; and (C) <i>S. aureus</i> forming no biofilm in CRA after treatment of GMM vapour.	107
61	Effect of MO treatment on <i>S. aureus</i> biofilm formation on glass test tubes.	107
62	Effect of GMM treatment on <i>S. aureus</i> biofilm formation on glass test tubes.	108
63	Vapour diffusion assay using MO and GMM against <i>P. aeruginosa</i> .	108
64	Microscopic assay using crystal violet for biofilm inhibition assay using GMM and MO against <i>P. aeruginosa</i> .	109
65	EPS inhibition assay using GMM and MO against <i>P. aeruginosa</i> .	109
66	Pyocyanin inhibition assay against <i>P. aeruginosa</i> using GMM and MO.	110
67	Vapour diffusion assay using MO and GMM against <i>Chromobacterium violaceum</i> .	110
68	Violacein inhibition assay using various concentrations of MO and GMM against <i>Chromobacterium violaceum</i> .	111
69	(A) Control plate with <i>C. albicans</i> ; antifungal assay against <i>C. albicans</i> using (B) MO; (C) optimized GMM using vapour diffusion method.	111
70	(A) Minimum inhibitory concentration of optimized GMM against <i>C. albicans</i> ; (B) streaking of the fungal colony from below the oil sample from the plate in (A) for determination of minimum fungicidal concentration. Note: 1 (GMM), 2(GMM/2), 3 (GMM/4), 4 (GMM/8), 5 (GMM/16), 6 (MO).	112

71	Zone of inhibition of optimized GMM against <i>C. albicans</i> during MIC determination. Note: NS- Not significant, ***- $p<0.001$.	112
72	Lactophenol blue staining of <i>C. albicans</i> treated with (A) GMM/8 dilution, (B) MO and (C) no treatment.	113
73	(A) Poison food assay against <i>C. albicans</i> using optimized GMM. Note: NS- Not significant, **- $p<0.01$, ***- $p<0.001$; (B) Line graph showing the inhibition of <i>C. albicans</i> by various concentrations of MO and GMM.	114
74	Showing the growth of <i>C. albicans</i> using various concentrations of MO and GMM during poison food assay after 48 hours of incubation.	114
75	(A) Scanning electron micrographs of <i>C. albicans</i> with a magnification of 5500X; (B) Scanning electron micrographs of <i>C. albicans</i> treated with MO (direct contact) with a magnification of 5500X; (C) Scanning electron micrographs of <i>C. albicans</i> treated with GMM/2 (0.50%, v/v) dilution (direct contact) with a magnification of 5500X; and (D) Scanning electron micrographs of <i>C. albicans</i> treated with GMM without dilution (direct contact) with magnification of 5500X.	115
76	Representation of 3D and 2D interaction of 1nmt with 3-vinyl dithiin.	116
77	Representation of 3D and 2D interaction of 1nmt with AITC.	117
78	Representation of 3D and 2D interaction of 1nmt with allicin.	117
79	Representation of 3D and 2D interaction of 1nmt with sinigrin.	117
80	Representation of 3D and 2D interaction of 1nmt with E-ajoene.	118
81	Representation of 3D and 2D interaction of 1nmt with 2-vinyl-dithiin.	118
82	Representation of 3D and 2D interaction of 1nmt with 1-butene-4-isothiocyanato.	118
83	Representation of 3D and 2D interaction of 1nmt with Z-ajoene.	119
84	Cytotoxicity activity of MO against HEK 293 cell, MCF7 and THP1 cell lines.	120
85	Cytotoxicity activity of GMM against HEK 293 cell, MCF7 and THP1 cell lines.	120
86	Relative gene expression of A. TNF- α , B. IL-1 β , C. IL-6, D. IL-8 and E. COX-2 checked by semi-quantitative PCR using gene-specific primers. The band intensities were quantitated and data are presented as mean \pm SEM of three independent experiments. One-way ANOVA and post hoc Bonferroni Comparison test were performed between control vs. LPS (#) and LPS vs. MO and GMM (*), representing statistical significance: ** $p<0.01$; *** $p<0.001$; ###, **** $p<0.0001$; and NS: Non-significant.	122
87	2D docking modes of (A) 1-butene-4-isothiocyanato; (B) 2-vinyl dithiin; (C) 3-vinyl dithiin; (D) Allyl isothiocyanate; (E) allicin; (F) E-ajoene; (G) Sinigrin; (H) Z ajoene with COX2 protein.	125
88	2D docking modes of (A) 1-butene-4-isothiocynato; (B) 2-vinyl dithiin; (C) 3-vinyl dithiin; (D) Allyl isothiocyanate; (E) allicin; (F) E-ajoene; (G) Sinigrin; (H) Z ajoene with IL-1 β .	126
89	2D docking modes of (A) 1-butene-4-isothiocynato; (B) 2-vinyl dithiin; (C) 3-vinyl dithiin; (D) Allyl isothiocyanate; (E) allicin; (F) E-ajoene; (G) Sinigrin; (H) Z ajoene with IL6.	127
90	2D docking modes of (A) 1-butene-4-isothiocynato; (B) 2-vinyl dithiin; (C) 3-vinyl dithiin; (D) Allyl isothiocyanate; (E) allicin; (F) E-ajoene; (G) Sinigrin; (H) Z ajoene with TNF alpha.	128

91	2D docking modes of (A) 1-butene-4-isothiocyano; (B) 2-vinyl dithiin; (C) 3-vinyl dithiin; (D) Allyl isothiocyanate; (E) allicin; (F) E-ajoene; (G) Sinigrin; (H) Z ajoene with IL8.	129
92	(A) Showing diffusion of MO through the eggshell membrane during and 2hr of incubation; (B) Showing diffusion of GMM through the eggshell membrane during and 2hr of incubation; (C) line graph showing the volume of oil diffused through the eggshell membrane during the 2hr incubation time.	131
93	Showing the FTIR results of the untreated eggshell membrane (black), MO treated membrane (red) and GMM treated membrane.	131
94	Liquid chromatogram of (A) diffused MO through an eggshell membrane after extraction in acetonitrile; (B) diffused MO through an eggshell membrane after extraction in acetonitrile.	132
95	Mass spectrometry plot of (A) GMM and (B) MO after diffusion through the eggshell membrane at a retention time of 2.77 minutes.	133
96	Mass spectrometry plot of (A) GMM and (B) MO after diffusion through the eggshell membrane at a retention time of 7.43 minutes.	134
97	Sensory acceptability test of GMM and MO in 30 volunteers. Bars with different alphabet labels in each group are significantly different ($P \leq 0.05$).	135

LISTS OF TABLES

Table No.	Title	Page No.
1	Details of the collection location of <i>Brassica nigra</i> seeds	29
2	The independent variables used during RSM represented Coded and uncoded format	38
3	Representing 17 different conditions for the garlic mustard oil macerate preparation designed by Central Composite Design.	38
4	Describing the parameters for preliminary GMM preparation	42
5	Details of the preparation method for GMM based on the ratio of garlic and mustard oil	42
6	Details of the preparation method for GMM based on the time of heating of GMM at 160°C	42
7	Details of the preparation method for GMM based on time of heating of GMM at 80°C	43
8	Sequence of the forward and reverse primers used for gene amplification	53
9	The details of the protein used for molecular docking, PDB code, grid box coordinate and size.	54
10	The proximate analysis of mustard (<i>Brassica nigra</i> L.) seeds and raw garlic (<i>Allium sativum</i> L.)	61
11	Showing the characteristic bonds and type for the observed peak for MO and GMM.	65
12	Details of antioxidant activity in terms of scavenging percentage and concentration (mM GAEAC) and the ratio of lipophilic and hydrophilic part of the hydrophilic part, lipophilic part, and whole oil of mustard oil and garlic mustard oil macerated	68
13	LCMS analysis of GTE, MO, and GMM	78
14	Major compounds of mustard oil and garlic mustard oil macerate identified by GCMS analysis.	79
15	Representing 17 different conditions for the garlic mustard oil macerate preparation designed by Central Composite Design along with the concentration of ajoene and 2-vinyl-4H-1,3, dithiin.	80
16	Representing the polynomial equation for the synthesis of ajoene ($\mu\text{g/ml}$ of GMM) (Y_1) and 2-vinyl-4H-1,3, dithiin ($\mu\text{g/ml}$ of GMM) (Y_2).	81
17	ANOVA of the quadratic model for the optimization of ajoene ($\mu\text{g/ml}$ of GMM) (Y_1) and 2-vinyl-4H-1,3, dithiin ($\mu\text{g/ml}$ of GMM) (Y_2).	82
18	Representing the predicted value and the experimental values of ajoene ($\mu\text{g/ml}$ of GMM) (Y_1) and 2-vinyl-4H-1,3, dithiin ($\mu\text{g/ml}$ of GMM) (Y_2).	83
19	Relative scoring of the antibacterial activity of prepared GMM based on the ratio of garlic and MO against <i>S. aureus</i>	86
20	Relative scoring of the antibacterial activity of prepared GMM based on time of heating against <i>S. aureus</i>	87
21	Qualitative estimation of antifungal activity of GMM based on the ratio of garlic and MO.	91
22	Qualitative estimation of antifungal activity of GMM heated for different times at 1600°C through vapour diffusion method.	92

23	The number of colonies of <i>C. albicans</i> after the treatment by prepared GMM heated for different times at 80°C through vapour diffusion method.	93
24	MIC and MBC against gram-positive and gram-negative bacteria	99
25	Showing binding energy and type of molecular interaction of the phytochemicals with the protein dehydroxysqualene synthase crtM.	103
26	Showing the binding energy, number of hydrogen bonds and type of interactions of selected molecules with N-myristoyltransferase (nmt, PDB ID: 1nmt) during molecular docking study	116
27	SwissADME analysis results of the volatile compounds present in garlic mustard oil macerate	123
28	Showing the binding energy of selected volatile molecules present in GMM with pro-inflammatory cytokines (COX-2, IL1 β , IL6, IL8, TNF α) during molecular docking study.	130

List of abbreviation

GMM	Garlic mustard oil macerate
GMM80	Garlic mustard oil macerate heated at 80°C
GMM160	Garlic mustard oil macerate heated at 160°C
AITC	allyl isothiocyanate
BITC	1-Butene, 4-isothiocyanato-
VD	2-vinyl-4H-1,3-dithiin
AJ	ajoene
DAS	Diallyl sulfide
DADS	Diallyl disulfide
DATS	Diallyl trisulfide
MO	Mustard oil
RSM	Response surface methodology
h	Hours
°C	Degree Celsius
VOC	Volatile organic compounds
SX	Staphyloxanthin
UV	Ultraviolet
FTIR	Fourier Transformed Infra-Red
SEM	Scanning electron microscopy
SA	<i>Staphylococcus aureus</i>
CA	<i>Candida albicans</i>
LPS	Lipopolysaccharide
IL-1 β	Interleukin-1 β
IL-8	Interleukin-8
Cox2	Cyclooxygenase-2
TNF- α	Tumor necrosis factor- α
IL-6	Interleukin-6
NO	Nitric oxide
PGE ₂	Prostaglandin E ₂
DAS	Diallyl sulfide
USDA	United States Department of Agriculture
TLC	Thin layer chromatography
HPLC	high-performance liquid chromatography
LCMS	Liquid chromatography-mass spectrometry
GCMS	Gas chromatography-mass spectrometry
OSCs	Organo-sulfur compounds
NSAIDs	Non-steroidal anti-inflammatory drugs
EPS	Extracellular polymeric substance
TDDS	Transdermal drug delivery system
Z-10-DA	Z-10-devinylajoene
FFA	Free fatty acid value
PV	Peroxide value
AV	Acid value
IV	Iodine value
SV	Saponification value

DPPH	2,2-diphenyl-1-picrylhydrazyl
LF	Lipophilic fraction
HF	Hydrophilic fraction
CCD	Central composite design
MIC	Minimum inhibitory concentration
MBC	Minimum bactericidal concentration
MFC	Minimum fungicidal concentration
PMNs	Polymorphonuclear leukocytes
QS	Quorum sensing
RNA	Ribonucleic acid
HSV1	Herpes simplex virus type 1
HSV2	Herpes simplex virus type 2
PV3	Parainfluenza virus type 3
VV	Vaccinia virus
HRV2	Human rhinovirus type 2
HIV	Human immunodeficiency virus
Mpro	Main protease
PLpro	Papain-like protease
SARS	Severe acute respiratory syndrome coronavirus 2
CoV-2	
mm Hg	Millimetres of mercury
g	Grams
N	Normality
M	Molarity
HCl	Hydrochloric acid
Na ₂ CO ₃	Sodium carbonate
H ₂ SO ₄	Sulfuric acid
AOAC	Association of Official Agricultural Chemists
rpm	Revolution per minutes
CH ₃ COOH	Acetic acid
CHCl ₃	Chloroform
Na ₂ S ₂ O ₃	Sodium thiosulfate
NaOH	Sodium hydroxide
KI	Potassium iodide
KBr	Potassium Bromide
PTFE	Polytetrafluoroethylene
eV	Electron volts
NIST	National Institute of Standards and Technology
MHA	Mueller Hinton Agar
MHB	Mueller Hinton Broth
SDA	Sabouraud dextrose agar
CFU	Colony forming unit
ANOVA	Analysis of variance
PBS	Phosphate buffer saline
RCSB	Research Collaboratory for Structural Bioinformatics
DMSO	Dimethyl sulfoxide
FBS	Fetal bovine serum
DMEM	Dulbecco's modified Eagle media
PMA	1-phorbol-12-myristate-13-acetate
RPMI	Roswell Park Memorial Institute

MTT	3- (4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide
SDS	Sodium dodecyl sulphate
nm	Nanometres
ADME	Absorption, Distribution, Metabolism and Excretion
HMO	Heated mustard oil
N.D.	Not detected
GMLF	Garlic mustard oil lipophilic fraction
GMHF	Garlic mustard oil hydrophilic fraction
MLF	Mustard oil lipophilic fraction
MHF	Mustard oil hydrophilic fraction
GAEAC	Gallic acid equivalence antioxidant capacity
GTE	Garlic toluene extract
TIC	Total ion current
3D	Three dimensions
ASN	Asparagine
ARG	Arginine
HIS	Histidine
ASP	Aspartame
GLY	Glycine
GLN	Glutamine
TYP	Tryptophane
THR	Threonine
LEU	Leucine
LYS	Lysine
VAL	Valine
CRA	Congo red agar
ZOI	Zone of inhibition
m/z	Mass by charge ratio
nmt	N-myristoyltransferase
BBB	Blood-brain barrier
Oligo dT	Deoxythymidine nucleotide
dNTP	Deoxynucleotide triphosphate
RT	Reverse transcription
DTT	Dithiothreitol
SAC	S-allyl cysteine
MUFA	Monounsaturated fatty acids