APPENDIX-I

LIST OF ABBREVIATIONS

$^{13}$C NMR: Carbon Nuclear Magnetic Resonance
$^{1}$H NMR: Proton/ Hydrogen Nuclear Magnetic Resonance
3D: 3 Dimensional
3D-QSAR: 3 Dimensional Quantitative Structure Activity Relationships
ADME/Tox: Absorption Distribution Metabolism Excretion and Toxicity
ALP: Alkaline Phosphatase
APCI: Atmospheric Pressure Chemical Ionization
ATP: Adenosine Triphosphate
CADD: Computer Aided Drug Design
CAT: Catalase
CCl$_4$: Carbon tetrachloride
CDCl$_3$: Deuterated Chloroform
CI: Chemical Ionization
DAS: Diacetyl Scopadol
DEPT: Distortionless Enhancement by Polarization Transfer
DFT: Density Functional Theory
DPPH: Diphenylpicrylhydrazyl
EA: Ethyl Acetate
EI-MS: Electron Ionization- Mass Spectrometry
ESI: Electrospray Ionization
FDA: Food and Drug Administration
FT-IR: Fourier Transform-Infared Spectroscopy
GC-MS: Gas Chromatography-Mass Spectrometry
GI: Gastro Intestinal
GPx: Glutathione Peroxidase
GSH: Glutathione
GST: Glutathione-S-Transferase
H+K-ATPase: Hydrogen Potassium ATPase
HASD: Hydroalcoholic extract of *Scoparia dulcis*
Hb: Hemoglobin
HBA: Hydrogen Bond Acceptor
HBD: Hydrogen Bond Donor
HIV: Human Immunodeficiency Virus
HIV: Human Immunodeficiency Virus
HMG-CoA: 3-hydroxy-3-methylglutaryl coenzyme A
HOMO: Highest Occupied Molecular Orbital
HPLC: High Performance Liquid Chromatography
HPX: Hydroperoxides
HSV-TK: Herpes Simplex Virus-Thymidine Kinase
IC: Inhibitory Concentration
IR: Infrared spectroscopy
LUMO: Lowest Unoccupied Molecular Orbital
M: Methanol
MALDI: Matrix Assisted Laser Desorption Ionization
MS: Mass Spectrometry
NCBI: National Center for Biotechnology Information
NGF: Nerve Growth Factor
NMR: Nuclear Magnetic Resonance
PCV: Packed Cell Volume
PDB: Protein Data Bank
PDM: Petroleum ether, Diethyl ether and Methanol
PE: Petroleum Ether
R & D: Research and Development
RBC: Red Blood Corpuscle
RCSB: Research Collaboratory for Structural Bioinformatics
*Rf*: Retention factor
RINm5F: Rat Insulinoma cell lines
RT: Reverse Transcriptase
SAC: *Scoparia dulcis* L. Acetone extract
SAD: Scoparic Acid D
SDB: Scopadulcic acid B
SDF: Structure Data Format
SDF7: *Scoparia dulcis* fraction-7
SEA: *Scoparia dulcis* L. Ethyl Acetate extract
SGOT: Serum Glutamate Oxaloacetate Transaminase
SGPT: Serum Glutamate Pyruvate Transaminase
SM: *Scoparia dulcis* L. Methanol extract
SOD: Superoxide Dismutase
SPE: *Scoparia dulcis* L. Petroleum Ether extract
SPEt: *Scoparia dulcis Plant Extracts*
STZ: Streptozotocin
TBARS: Thiobarbituric Acid Reactive Substances
TLC: Thin Layer Chromatography
TPA: Tumor Promoter 12-O-tetradecanoylphorbol-13-acetate
VS: virtual screening
wwPDB: Worldwide Protein Data Bank
APPENDIX-II

PREPARATION OF REAGENTS

a) Mayer's reagent

1.358 gram of mercuric chloride was dissolved in 60 ml of distilled water. 5 gram of potassium iodide was dissolved in 10 ml of water. The two solutions were then mixed and diluted with water to make the volume 100 ml.

b) Fehling's solution

- Fehling's solution-A: 6.93 gram of CuSO4.5H2O was dissolved in 100 ml distilled water.
- Fehling's solution-B: 0.44 gram of sodium potassium tartrate and 13.0 gram of NaOH was dissolved in 100 ml distilled water.

c) Preparation of Ferric chloride solution (0.5M, 1.5 N)

135.2 gram FeCl3.6H2O was dissolved in 20 ml conc. HCl and was diluted using distilled water to make the volume 1 litre.
APPENDIX-III

DATABASES, SOFTWARE AND SERVERS

a) ACD Chemsketch (http://www.acdlabs.com/resources/freeware/chemsketch/)
b) BindingDB (www.bindingdb.org)
c) ChEMBL (https://www.ebi.ac.uk/chembldb/)
d) Drugbank (http://www.drugbank.ca)
e) HyperChem
   (http://www.hyper.com/Products/HyperChemProfessional/tabid/360/Default.aspx)
f) LeadIT FlexX (http://www.biosolveit.de/LeadIT/)
g) Mobyle@RPBS (http://mobyle.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py)
h) Molsoft (http://www.molsoft.com)
i) Open Babel (http://openbabel.org/wiki/Main_Page)
j) PDBsum (https://www.ebi.ac.uk/pdbsum)
k) Perkin Elmer ChemOffice 2012
l) Protein Data Bank (www.rcsb.org/pdb)
o) Q-SiteFinder (http://www.modelling.leeds.ac.uk/qsitefinder/)
p) ReverseScreen3D (www.modelling.leeds.ac.uk/ReverseScreen3D/)
APPENDIX-IV

LIST OF PUBLICATIONS

RESEARCH PAPERS:


5. Saikia, R., Chetia, P., Talukdar, A. D., Choudhury, S. and Choudhury, M. D. Computational Therapeutic Screening of a Novel Metabolite (E)-7-methyl-2-(5,6,7,8-tetrahydronaphthalen-2-yl)oct-5-en-3-one Isolated from *Scoparia dulcis* L. *Combinatorial chemistry and high throughput screening.* (Under review).
BOOK CHAPTER:

APPENDIX-V

HERBARIUM OF SCOPARIA DULCIS L.