CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

Editors:
Ibrahim Ali Noorbatcha
Hamzah Mohd. Salleh
Mohamed Elwathig Saeed Mirghani
Raha Ahmad Raus

IIUM PRESS
INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA
CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

(VOLUME II)

Editors:
Ibrahim Ali Noorbatcha
Hamzah Mohd. Salleh
Mohamed Elwathig Saeed Mirghani
Raha Ahmad Raus

Department of Biotechnology Engineering
Faculty of Engineering
International Islamic University Malaysia

IIUM Press
CONTENTS

PREFACE

CHAPTER 1 SCREENING FOR ANTI-CANCER COMPOUND FROM SELECTED MALAYSIAN PLANTS BY SULFORHODAMINE B ASSAY ON MCF-7 CANCER CELL LINE
Azura Amid, Abdul Aziz Ahmad and Raha Ahmad Raus

CHAPTER 2 THE EVALUATION ON ANTICANCER PROPERTIES FROM KENAF SEEDS OIL FROM DIFFERENT VARIETIES
Azura Amid, Parveen Jamal, Nurul Elyani Mohamad and Engku Hasnah Engku Abdullah

CHAPTER 3 SCREENING AND EVALUATION OF ANTICANCER PROPERTY IN MANGO FRUIT Mangifera indica
Azura Amid, Irwandi Jaswir and Muhd. Ezza Faiez Othman

CHAPTER 4 SENSORY EVALUATION AND CONTAMINATION TEST ON MANGO FRUIT Mangifera indica PUREE
Azura Amid, Irwandi Jaswir and Muhd. Ezza Faiez Othman

CHAPTER 5 THE OBSERVATION ON THE INHIBITION OF ANTI-INFLAMMATORY MEDIATOR OF THE TOMATO LEAVES EXTRACT
Azura Amid, Sulawati Semail and Parveen Jamal

CHAPTER 6 A STUDY OF BACTERIAL CELL IMMOBILIZATION IN ALGINATE GEL BEADS FOR THE PRODUCTION OF MYO-INOSITOL PHOSPHATES
Noor Illi Mohamad Puad, Abd-ElAzim Farouk and Hamzah Mohd. Salleh

CHAPTER 7 EXTRACTION AND EVALUATION OF ANTIBACTERIAL ACTIVITY FROM SELECTED FLOWERING PLANTS
Raha Ahmad Raus, Erlina Abdullah and Parveen Jamal
CHAPTER 8  EXTRACITION OF ANTIBACTERIAL COMPOUNDS FROM PLANTS USING SONICATOR  
Raha Ahmad Raus, Nur Shazwana Mohd Puzi and Parveen Jamal  

CHAPTER 9  EXTRACITION AND EVALUATION OF ANTICANDIDAL ACTIVITY FROM SELECTED MALAYSIAN PLANTS  
Raha Ahmad Raus, Nor Azlin Alia Nor Muhammad and Jacinta Santhanam  

CHAPTER 10  EXTRACITION AND EVALUATION OF ANTIFUNGAL ACTIVITY FROM SELECTED MALAYSIAN PLANTS  
Raha Ahmad Raus, Hayatunissa Samsuddin, Nor Hafizah Addnan and Jacinta Santhanam  

CHAPTER 11  MOLECULAR MODELING OF BIODEGRADATION POLYESTERS USING LIPASE  
Ibrahim Ali Noorbatcha, Nor Afina Eidura Hussin and Hamzah Mohd Salleh  

CHAPTER 12  POTENTIAL OF NAHAR SEED OIL EXTRACT AS ANTIMICROBIALS  
Mohamed E. S. Mirghani, I. A. Ahmed, S. A. Muyibi., J. I. Daoud and M. A. Mikail  

CHAPTER 13  NAHAR (Mesua ferrea) TREE AS A MEDICINAL PLANT  
Mohamed E. S. Mirghani, I. A. Ahmed, S. A. Muyibi., J. I. Daoud and M. A. Mikail  

CHAPTER 14  EXPLOIT OF MALAYSIAN MANGO KERNEL EXTRACT AS ANTIBACTERIAL AGENT  
Mohamed Elwathig Saeed Mirghani, Nasereldin A. Kabbashi, Parveen Jamal and H. A. Abdullah  

CHAPTER 15  PREPARATION OF NUTRITIOUS DRINK FROM DATE PALM KERNEL (DPK)  
Mohamed Elwathig Saeed Mirghani, Irwandi Jasir and Nurul Hanan Mustapha  

CHAPTER 16  DATE SEED EXTRACT AS PRESERVATIVES  
Mohamed E. S. Mirghani, M. A. Mikail, I. A. Ahmed, M. I. Abdul Karim and J. I. Daoud
CHAPTER 17 IMMOBILIZATION OF LIPASE BY CROSS-LINKED ENZYME AGGREGATE (CLEA) TECHNOLOGY
Faridah Yusof and Nik Rashidah Nik Abdul Ghani

CHAPTER 18 DETECTION OF ETHANOL IN BEVERAGES USING AN ELECTRONIC NOSE
Irwandi Jaswir, Nurul Asyikeen A.M and Rini Akmeliawati

CHAPTER 19 EFFECTS OF CELL IMMOBILIZATION TO THE PHYTATE-DEGRADING ENZYME ACTIVITY
Noor Illi Mohamad Puad, Abd-ElAzim Farouk and Hamzah Mohd. Salleh

CHAPTER 20 ENZYMATIC DEVULCANIZATION OF WASTE RUBBER
Faridah Yusof and Ainie Asyikin Ahmad

CHAPTER 21 EXTRACTION AND CHARACTERIZATION OF ASTAXANTHIN FROM MARINE SOURCES
Irwandi Jaswir, Shazana Azfar and Azura Amid

CHAPTER 22 EXTRACTION OF FISH COLLAGEN USING ENZYMATIC PROCESS
Irwandi Jaswir, Noor Yuslida Hazahari and Mohamed Elwathig Saeed Mirghani

CHAPTER 23 FROM RECREATION MATHEMATICS TO PSEUDO-GENES
Ibrahim Ali Noorbachta and Ahmad Faizul Shamsudin

CHAPTER 24 MECHANICAL PROPERTIES OF A GELATIN REPLACER, PECTIN, FROM BANANA AND MANGO PEELS
Hamzah Mohd. Salleh, Irwandi Jaswir and Hamida Zakaria

CHAPTER 25 DEVELOPMENT OF IN-VIVO BIOFUEL CELL FOR IMPLANTABLE MEDICAL DEVICES
Hamzah Mohd. Salleh, Nur Syaheera Mohd Yusoff, Raihan Othman and Mohd. Firdaus Abd. Wahab

CHAPTER 26 IMPROVEMENT OF EXTRACTION PROCESSING CONDITIONS FOR ANTIBACTERIAL COMPOUNDS FROM Curcuma longa
CHAPTER 27  IMPROVEMENT OF SONICATION PROCESSING CONDITIONS FOR EXTRACTION OF ANTIBACTERIAL COMPOUNDS FROM Spathiphyllum cannifolium

Raha Ahmad Raus, Nur Shazwana Mohd Puzi and Parveen Jamal

CHAPTER 28  IMPROVING ENZYME CATALYSIS THROUGH THE IMPROVEMENT OF BINDING STRENGTH: SIMULATED MUTATION TO PREDICT THE MUTATIONAL EFFECT ON XYLANASE CEX

Ibrahim Ali Noorbatha, Muaz Abdul Hadi, Ahmad Faris Ismail and Hamzah Mohd Salleh

CHAPTER 29  MOLECULAR INTERACTION ANALYSIS TO DESIGN NEW DRUG CANDIDATES FOR LYSOSOMAL STORAGE DISEASE

Ibrahim Ali Noorbatha, Muaz Abdul Hadi, Zarul Azwan Adam and Hamzah Mohd Salleh

CHAPTER 30  MECHANICAL IMPROVEMENT OF HALAL GELATIN FROM MARINE SOURCES

Irwandi Jaswir, Aniza Binti Asari and Hamzah Mohd. Salleh

CHAPTER 31  PERFORMANCE OF ARTIFICIAL ANTIOXIDANTS IN RBD PALM OLEIN DURING DEEP-FAT FRYING

Irwandi Jaswir and Ahmad Badli Yusoff

CHAPTER 32  PHYSICO-CHEMICAL PROPERTIES OF COLLAGEN EXTRACTS FROM TWO LOCAL FISH SPECIES

Irwandi Jaswir, Nur'a'ain Che Kamaludin and Hamzah Mohd. Salleh

CHAPTER 33  PHYTOCHEMICAL SCREENING AND PURIFICATION OF XOI FROM SELECTED MEDICINAL PLANT

Parveen Jamal, Azura Amid and Suhana Abdullah

CHAPTER 34  POTENTIAL ENERGY SURFACES FOR REACTIONS AMONG HYDROGEN FLUORIDE MOLECULES

Ibrahim Ali Noorbatha, Borhanuddin Ariffin and Sharifudin M Zain
CHAPTER 35 POTENTIAL REMEDIES FOR GOUT FROM MEDICINAL PLANTS
Parveen Jamal, Saiful Mohammad Nizam Azmi and Azura Amid

CHAPTER 36 PRODUCTION OF CARRAGEENAN FROM MALAYSIAN SEAWEED
Irwandi Jaswir, Ainur Farhana and Parveen Jamal

CHAPTER 37 PRODUCTION OF GELATIN REPLACERS FROM MALAYSIAN TUBEROUS PLANTS
Irwandi Jaswir, Nurul Ain Zafirah Binti Kamalurudin and Hamzah Mohd. Salleh

CHAPTER 38 PURIFICATION OF PATATIN-LIKE PROTEIN (HEV B7) FROM SKIM LATEX OF Hevea brasiliensis
Faridah Yusof and Nurul Ain Harmiza Abdullah

CHAPTER 39 PURIFICATION OF SUPEROXIDE DISMUTASE FROM Hevea brasiliensis LEAF EXTRACT
Faridah Yusof and Nazhirah Mohamed

CHAPTER 40 QUALITATIVE AND QUANTITATIVE ANALYSIS OF ANTI-GOUT FROM Carica papaya LEAVES
Parveen Jamal, Saiful Mohammad Nizam Azmi and Azura Amid

CHAPTER 41 RECYCLING OF WASTE RUBBER VIA MICROBIAL DEVULCANIZATION
Faridah Yusof and Aini Asyikin Ahmad

CHAPTER 42 SCREENING ANTI-CANCER COMPOUNDS FROM PALM OIL INDUSTRIAL WASTES
Raha Ahmad Raus, Syamsa Shazwan Shamsudin and Parveen Jamal

CHAPTER 43 SCREENING ANTI-CANCER COMPOUNDS FROM MEDICINAL MALAYSIAN PLANTS
Raha Ahmad Raus, Yusuf Johari and Azura Amid

CHAPTER 44 SCREENING ANTI-CANCER COMPOUNDS FROM RICE INDUSTRIAL WASTES
Raha Ahmad Raus, Mohd Haftizul Muhammad and Parveen Jamal
CHAPTER 45 SOLUBILIZATION OF VITAMIN E IN CULTURE MEDIUM AND ITS ANTIOXIDANT ACTIVITY
Irwandi Jaswir and Siti Fairus Sahul Hamid

CHAPTER 46 STRUCTURE ACTIVITY RELATIONS IN PENTACYCLIC TRITERPENOIDS TOWARDS HYALURONIDASE INHIBITORY ACTIVITY
Ibrahim Ali Noorbatha, Nor Hayati Abdullah and Khalijah Awang

CHAPTER 47 IN SILICO PREDICTION OF ANTICANCER ACTIVITY OF NITROSOUREAS

CHAPTER 48 BIOMOLECULAR COMPUTING IN DEGENERATIVE BRAIN RESEARCH
Ibrahim Ali Noorbatha and Ahmad Faizul Shamsudin

CHAPTER 49 ISOLATION AND IDENTIFICATION OF FERULIC ACID FROM RICE BRAN
Faridah Yusof and Aimi Izyana Ismail

CHAPTER 50 IMPROVEMENT OF EXTRACTION PROCESSING CONDITIONS FOR ANTIFUNGAL COMPOUNDS FROM Alpinia galanga
Raha Ahmad Raus, Nor Hafizah Addnan, Norha Mat Amin and Syamsiah Aini Shohaimi

xi
CHAPTER 28

IMPROVING ENZYME CATALYSIS THROUGH THE IMPROVEMENT OF BINDING STRENGTH: SIMULATED MUTATION TO PREDICT THE MUTATIONAL EFFECT ON XYLANASE CEX

Ibrahim Ali Noorbatches\textsuperscript{1}, Muaz Abdul Hadi\textsuperscript{1}, Ahmad Faris Ismail\textsuperscript{2} and Hamzah Mohd. Salleh\textsuperscript{1}

\textsuperscript{1}Department of Biotechnology Engineering,  \\Department of Mechanical Engineering,  
Faculty of Engineering,  
International Islamic University Malaysia, P.O. Box 10, 50728 Kuala Lumpur, Malaysia

ABSTRACT

Xylanase enzymes are extensively used in biobleaching in the industry including paper and detergent industry. Hence the enhancement of their functional properties can give significant boost to this industry. Through this project, multiple trials have been conducted to suggest mutations to improve the properties of Xylanase enzyme family 10 from \textit{Cellulomonas fimi}. The simulated mutation using Computer Aided Mutation (CAM) suggests enhancements in term of the binding strength that may lead to better catalysis reaction. The double point mutation of K47R and Q87N was found to increase binding of the ligands in the active site. Automated ligand docking analysis is used to demonstrate how different mutations can improve the binding strength of xylanase CeX. These results can be used to predict mutations that will improve the catalytic strength of the enzymes which can be used as a starting point for experimental studies.

\textit{Keywords}: xylanase CeX, xylanase mutation, \textit{Cellulomonas fimi}, computer aided design

INTRODUCTION

Xylanases are enzymes that catalyze the degradation of xylan, the main component of hemicellulose (Honda et al., 2091). Their biotechnological applications are of interest to the animal-feed, food-processing, and pulp-and-paper industries (Shibuya, 2000). In particular, xylanase has been found to be effective in reducing chlorine dosage requirements in the Kraft pulp-bleaching process (Viikari et al., 1994). Xylanase Cex is one of the xylanase enzymes from glycosyl hydrolase Family 10 (GH 10) (Davies, et al., 1995). It is from bacterium, Cellulomonas fimi and undergoes retaining mechanism. The active site nucelophile is Glu 233 (Tull et al., 1991) and the acid base catalyst is Glu 127 (MacLeod, 1994). In term of economical overview, for example in pulp industries (Suurnaki, 1996), the use of xylanase to degrade xylan is more beneficial compared to use of chemical processes which are expensive and cause environmental