

Biotechnologies towards Sustainable Development in Malaysia

Zarina Zainuddin

**IIUM PRESS
INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA**



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HUM Press

Published by:
IIUM Press
International Islamic University Malaysia

First Edition, 2011
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Perpustakaan Negara Malaysia

Cataloguing-in-Publication Data

Zarina Zainuddin

Biotechnologies towards Sustainable Development in Malaysia

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Include index

Bibliography: p. 149

ISBN: 978-967-418-200-7

Member of Majlis Penerbitan Ilmiah Malaysia – MAPIM
(Malaysian Scholarly Publishing Council)

Printed by :
IIUM PRINTING SDN. BHD.
No. 1, Jalan Industri Batu Caves 1/3
Taman Perindustrian Batu Caves
Batu Caves Centre Point
68100 Batu Caves
Selangor Darul Ehsan

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Chapter 10

Identifying catalytic residues for peptidases: *in silico* perspective

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Introduction

Proteases are involved in numerous aspects of the biogenesis and maintenance of bacteria, from the removal and degradation of signal sequences, through the degradation of partially assembled complexes or damaged proteins and adaptation to changes in environmental conditions. Identification of catalytic residues using experimental methods is most accurate. Unfortunately, experimental functional characterization is time-consuming and expensive. Furthermore they are not efficient enough to handle the rapidly accumulating protein sequences and structural data. Therefore, high-throughput *in silico* methods for identifying catalytic residues and peptidase function prediction are much needed.

The most commonly used method relies on the transfer of annotation from a characterised homologue, identified by sequence and structural similarity. Two major approaches for prediction of functional domains including catalytic reactions. The first approach is based solely on the protein sequence and evolutionary information from the multiple sequence alignments. This approach resulting the phylogenetic motifs, conserved blocks from the multiple sequence alignment, which later can be used to predict functional regions surrounding catalytic sites. Integration of sequence conservation information, predicted secondary structure and