

Florentino Fdez-Riverola  
Mohd Saberi Mohamad  
Miguel Rocha · Juan F. De Paz  
Pascual González *Editors*

Practical Applications of  
Computational Biology  
and Bioinformatics,  
12th International  
Conference

 Springer

*Practical Applications of Computational Biology and Bioinformatics*

12th International Conference (PACBB 2018)

Editors: Florentino Fdez-Riverola, Mohd Saberi Mohamad, Miguel Rocha, Juan F. De Paz,  
Pascual González

ISSN 2194-5357

ISSN 2194-5365 (electronic)

Advances in Intelligent Systems and Computing

ISBN 978-3-319-98701-9

ISBN 978-3-319-98702-6 (eBook)

<https://doi.org/10.1007/978-3-319-98702-6>

Library of Congress Control Number: 2018954643

© Springer Nature Switzerland AG 2019

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG  
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

---

## Contents

<b>A Hybrid of Simple Constrained Artificial Bee Colony Algorithm and Flux Balance Analysis for Enhancing Lactate and Succinate in <i>Escherichia Coli</i> . . . . .</b>	<b>1</b>
Mei Kie Hon, Mohd Saberi Mohamad, Abdul Hakim Mohamed Salleh, Yee Wen Choon, Muhammad Akmal Remli, Mohd Arfian Ismail, Sigeru Omatsu, and Juan Manuel Corchado	
<b>Parameter Estimation of Essential Amino Acids in <i>Arabidopsis thaliana</i> Using Hybrid of Bees Algorithm and Harmony Search . . . . .</b>	<b>9</b>
Mei Yee Aw, Mohd Saberi Mohamad, Chuii Khim Chong, Safaai Deris, Muhammad Akmal Remli, Mohd Arfian Ismail, Juan Manuel Corchado, and Sigeru Omatsu	
<b>In Silico Modeling and Simulation Approach for Apoptosis Caspase Pathways . . . . .</b>	<b>17</b>
Pedro Pablo González-Pérez and Maura Cárdenas-García	
<b>Molecular Dynamic Simulations Suggest that P152R Mutation Within MeCP2 Can Lead to Higher DNA Binding Affinity and Loss of Selective Binding to Methylated DNA . . . . .</b>	<b>27</b>
Dino Franklin	
<b>Impact of Genealogical Features in Transthyretin Familial Amyloid Polyneuropathy Age of Onset Prediction . . . . .</b>	<b>35</b>
Maria Pedroto, Alípio Jorge, João Mendes-Moreira, and Teresa Coelho	
<b>Feature Selection and Polydispersity Characterization for QSPR Modelling: Predicting a Tensile Property . . . . .</b>	<b>43</b>
Fiorella Cravero, Santiago Schustik, María Jimena Martínez, Carlos D. Barranco, Mónica F. Diaz, and Ignacio Ponzoni	

# A Hybrid of Simple Constrained Artificial Bee Colony Algorithm and Flux Balance Analysis for Enhancing Lactate and Succinate in *Escherichia coli*

Mei Kie Hon<sup>1</sup>, Mohd Saberi Mohamad<sup>2,3,✉</sup>,  
Abdul Hakim Mohamed Salleh<sup>1</sup>, Yee Wen Choon<sup>1</sup>,  
Muhammad Akmal Remli<sup>1</sup>, Mohd Arfian Ismail<sup>4</sup>, Sigeru Omatsu<sup>5</sup>,  
and Juan Manuel Corchado<sup>6</sup>

<sup>1</sup> Artificial Intelligence and Bioinformatics Research Group,  
Faculty of Computing, Universiti Teknologi Malaysia,  
81310 Skudai, Johor, Malaysia  
(mkhon4, ywchoon2)@live.utm.my,  
abdulkhakim.utm@gmail.com, akmalmuhd@gmail.com

<sup>2</sup> Institute for Artificial Intelligence and Big Data, Universiti Malaysia Kelantan,  
City Campus, Pengkalan Chepa, 16100 Kota Bharu, Kelantan, Malaysia

<sup>3</sup> Faculty of Bioengineering and Technology, Universiti Malaysia Kelantan,  
Jeli Campus, Lotk Bag 100, 17600 Jeli, Kelantan, Malaysia  
sabe@umk.edu.my

<sup>4</sup> Soft Computing and Intelligent System Research Group, Faculty of Computer  
Systems and Software Engineering, Universiti Malaysia Pahang,  
26300 Kuantan, Pahang, Malaysia  
arfian@ump.edu.my

<sup>5</sup> Department of Electronics, Information and Communication Engineering,  
Osaka Institute of Technology, Osaka 535-8585, Japan  
oma.tu@rsh.oit.ac.jp

<sup>6</sup> Biomedical Research Institute of Salamanca/BISITE Research Group,  
University of Salamanca, Salamanca, Spain  
corchado@usal.es

**Abstract.** In the past decades, metabolic engineering has received great attention from different sectors of science due to its important role in enhancing the over expression of the target phenotype by manipulating the metabolic pathway. The advent of metabolic engineering has further laid the foundation for computational biology, leading to the development of computational approaches for suggesting genetic manipulation. Previously, conventional methods have been used to enhance the production of lactate and succinate in *E. coli*. However, these products are always far below their theoretical maxima. In this research, a hybrid algorithm is developed to seek optimal solutions in order to increase the overproduction of lactate and succinate by gene knockout in *E. coli*. The hybrid algorithm employed the Simple Constrained Artificial Bee Colony (SCABC) algorithm, using swarm intelligence as an optimization algorithm to optimize the objective function, where lactate and succinate productions are maximized by simulating gene knockout in *E. coli*. In addition, Flux Balance