

3rd International Conference on Computation for Science and Technology 2014

(ICCST-3)

Advances in Computer Science Research Volume 5

**Bali, Indonesia
23-25 September 2014**

Editor:

Daryono H. Tjahjono

ISBN: 978-1-63439-973-9

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2014) by Atlantis Press
All rights reserved.
<http://www.atlantis-press.com/php/pub.php?publication=iccst-15>

Printed by Curran Associates, Inc. (2015)

For permission requests, please contact Atlantis Press
at the address below.

Atlantis Press
29 avenue Laumière
75019 Paris
France

contact@atlantispress.com

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

Molecular Docking and Molecular Dynamics Simulation of the Interaction of Cationic Imidazolium Porphyrin-Anthraquinone and Hsp90	1
<i>Muhammad Arba, Rahmana Emran Kartasasmita, Daryono H. Tjahjono</i>	
In Silico Study of The Component of <i>Eleutherine americana</i> MERR. on Human Estrogen Reseptor Alpha as Potential Anti-Breast Cancer	6
<i>Tasia Amelia, Dina Pratiwi, Romsiah, Daryono H. Tjahjono</i>	
Pyrazolylporphyrin Derivatives as New Potential Ligand for Melanoma Cancer Radiopharmaceutical Kit: In Silico Study	10
<i>Fransiska Kurniawan, Rahmana Emran Kartasasmita, Daryono H. Tjahjono</i>	
Complexes Formation of Porphyrin Derivatives with Lead: Preliminary Computational Study of Porphyrin as Analytical Reagent	16
<i>Rimadani Pratiwi, Slamet I. Surantaatmadja, Daryono H. Tjahjono</i>	
Interactions of Porphyrin-Acridine Hybrids to DNA Duplexes and Quadruplex: In Silico Study	20
<i>Hubbi Nashrullah Muhammad, Sophi Damayanti, Daryono H. Tjahjono</i>	
Toxicity Prediction of meso-5,15-di[3,4-bis(carboxymethylenoxy)phenyl] porphyrin and meso-5,15-di[3,4-bis(carboxymethylenoxy)phenyl],10,20-diphenyl porphyrin	25
<i>Fauzan Zein Muttaqin, Slamet I. Surantaatmadja, Abdul Mutalib, Daryono H. Tjahjono</i>	
Absorption, Distribution and Toxicity Prediction of Curculigoside A and its Derivatives	32
<i>Nursamsiar, Slamet I. Surantaatmadja, Daryono H. Tjahjono</i>	
In Silico Study of Andrographolide as Protease Inhibitors for Antimalarial Drug Discovery	36
<i>Sandra Megantara, Jutti Levita, Slamet I. Surantaatmadja</i>	
Study on CCR5 Receptor Antagonists as an Anti-Prostate Cancer: Inhibition Activity, QSAR and Molecular Docking	40
<i>Nursamsiar, Lina Nurfadhila, Iman S. Pratama, Aiyi Asnawi, Slamet I. Surantaatmadja</i>	
Acetylation of Asiatic Acid and Its Hepatotoxicity Prediction	45
<i>Ida Musfiroh, Ita Puspitasari, Ahmad Muhtadi, Rahmana Emran Kartasasmita, Slamet I. Surantaatmadja</i>	
Prediction of Hazard Identification and Characterization of Several Compounds used as Food Additives Applying In Silico Methods	49
<i>Ilitizam Nasrullah, Rahmana Emran Kartasasmita, Sophi Damayanti</i>	
Discovering Inhibitors of Tyrosinase Enzyme from Zingiberaceae for Depigmentation Agents	59
<i>Karina Muthia, Fride Rindu Alami, Nyi Mekar Saptarini, Jutti Levita</i>	
Computational Design of Dengue Type-2 NS2B/NS3 Protease Inhibitor: 2D/3D QSAR of Quinoline and Its Molecular Docking	63
<i>Maywan Hariono, Ezatul E. Kamarulzaman, Habibah A. Wahab</i>	
Docking of Dengue NS2B-NS3 Protease with <i>Murraya koenigii</i>	82
<i>Kai Sing Yong, Sy Bing Choi, Habibah A. Wahab</i>	
Molecular Dynamics Simulation on Designed Antibodies of HIV-1 Capsid Protein (p24)	85
<i>Hana Atiqah Abdul Karim, Chatchai Tayapiwatana, Piyyarat Nimmanpipug, Sharifuddin M. Zain, Noorsaadah Abd Rahman, Vannajan Sanghiran Lee</i>	
Computer-aided Structure-based Design of 3,3'-Diallyl-[1,1'-biphenyl]- 4,4'- diol Analogs of Eugenol as Potential Ligands for Estrogen Receptor Alpha	89
<i>Enade Perdana Istyastono, Yulia Anita, Andini Sundowo</i>	
Computational Alanine Scanning Mutagenesis: Characterizing the hotspots of ILK-Ankyrin Repeat and PINCH1 Complex	92
<i>Vertika Gautam, Nadia Hanim Sabri, Wei Lim Chong, Sharifuddin M. Zain, Noorsaadah Abd. Rahman, Vannajan Sanghiran Lee, Anand Gaurav</i>	
Molecular Docking Studies of Flavonoids of Noni Fruit (<i>Morinda citrifolia</i> L.) to Peroxisome Proliferator-Activated Receptor-Gamma (PPARγ)	95
<i>Fikry Awaluddin, Andrianopsyah Mas Jaya Putra, Supandi Supandi</i>	
Exploration of Residue Binding Energy of Potential Ankyrin for Dengue Virus II from MD Simulations	100
<i>Wei Lim Chong, Sharifuddin M. Zain, Noorsaadah Abd. Rahman, Rozana Othman, Shatrah Binti Othman, Piyyarat Nimmanpipug, Chatchai Tayapiwatana, Vannajan Sanghiran Lee</i>	
Binding Models of Polyphenols to Cytochrome P450 2C9: A Molecular Docking Study	104
<i>Siripat Chaichit, Darunee Hongwiset, Supat Jiranusornkul</i>	

Virtual Screening of 2-hydroxy-1,4-naphthoquinone Derivatives as Antimitotic Agent using Molegro Virtual Docker on Polo Like Kinase 1	108
<i>Susi Kusumaningrum, Soleh Kosela, Wahono Sumaryono, Emil Budianto, Alfian Danny Arbianto</i>	
QSAR Study of Quinazoline Derivatives as Inhibitor of Epidermal Growth Factor Receptor-Tyrosine Kinase (EGFR-TK)	114
<i>La Ode Aman, Widisusanti Abdulkadir, Julitha Geybie Rembet, Daryono H. Tjahjono</i>	
Cembranoid Diterpenes as Antitumor: Molecular Docking Study to Several Protein Receptor Targets	120
<i>Muhammad S. Zubair, Syariful Anam, Khalid O. Al-Footy, Ahmed Abdel-Lateef, Walied M. Alarif</i>	
Numerical Analysis on the Stability Behavior of a Dynamical System on the Deposit and Loan of a Bank	125
<i>Novriana Sumarti, H. Fansuri</i>	
Implementation of Finite Field Arithmetic Operations for Polynomial and Normal Basis Representations	129
<i>Mirza Maulana, Wenny Franciska Senjaya, Budi Rahardjo, Intan Muchtadi-Alamsyah, Marisa W. Paryasto</i>	
Reducing Computational Complexity of Network Analysis using Graph Compression Method for Brand Awareness Effort	135
<i>Andry Alamsyah, Yahya Peranginangin, Budi Rahardjo, Intan Muchtadi-Alamsyah, Kuspriyanto</i>	
Construction of θ-Cyclic Codes over an Algebra of Order 4	141
<i>Irwansyah, Intan Muchtadi-Alamsyah, Aleams Barra, Ahmad Muchlis, Djoko Supriyanto</i>	
Investigation of H(2H) - Pt(111) Interaction System: using Density Functional Methods	144
<i>Can Dogan Vurdu, Muhammet Serdar Cavus, Fatma Kandemirli</i>	
The Quantum Chemical Calculations of Some Thiazole Derivatives	149
<i>Murat Saracoglu, Fatma Kandemirli, Mohammed A. Amin, Can Dogan Vurdu, Muhammet Serdar Cavus, Gokhan Say ner</i>	
Model Identification of Continuous Fermentation under Noisy Measurements	155
<i>Rudy Agustriyanto</i>	
Surface Interaction between Ethylene, Hydroxide Ion, and Titanium Dioxide Anatase (001): A First Principle Density Functional Theory Study	158
<i>Paulus Himawan, Mohammad Kemal Agusta, Hermawan Kresno Dipojono, Ganes Shukri, Nugraha</i>	
Modeling of Dirac Electron Tunneling Current in Bipolar Transistor Based on Armchair Graphene Nanoribbon Using a Transfer Matrix Method	164
<i>Endi Suhendi, Rifky Syariati, Fatimah A. Noor, Neny Kurniasih, Khairurrijal</i>	
Acceleration of norm-conserving Pseudopotential Plane-Wave-Based DFT Calculation on GPU using CUDA	167
<i>F. Fathurahman, Enngar Alfianto, H. K. Dipojono, M. A. Martoprawiro</i>	
Artifacts Removal of EEG Signals using Adaptive Principal Component Analysis	171
<i>Arjon Turnip, Dwi Esti Kusumandari</i>	
Structural Study of Chalcogenide Material Ge-Te-Ga using <i>ab Initio</i> Molecular Dynamics	175
<i>Lilin Lalita, H. K. Dipojono, M. A. Martoprawiro</i>	
Author Index	