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HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH : PROSIDING

Judul Karya Ilmiah : Probing the interaction between EC1-EC2 domain of E-cadherin with conformational structure of cyclic ADTC7 (Ac-CDTPDC-NH₂) peptide using molecular docking approach

Jumlah Penulis : 7 Orang

Status Pengusul : Penulis ke-1

Identitas Prosiding :

- a. Judul Prosiding : Journal of Physics: Conference Series: The 9th International Seminar on New Paradigm and Innovation on Natural Sciences and Its Application (INSPINSA) 2019
- b. ISBN/ISSN : 978-1-5108-6265-4 / 1757-8981
- c. Thn Terbit, Tempat Pelaks. : 2020, Semarang – Indonesia
- d. Penerbit/Organiser : IOP Publishing Ltd
- e. Alamat Repository/Web : <https://iopscience.iop.org/issue/1742-6596/1524/1>
 Alamat Artikel : <https://iopscience.iop.org/article/10.1088/1742-6596/1524/1/012081/meta>
- f. Terindeks di (jika ada) : Scopus/Scimagojr/SJR = 0,23 (2019)

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 (beri ✓ pada kategori yang tepat) ☐ Prosiding Forum Ilmiah Nasional

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	Internasional ☐	Nasional ☐	
a. Kelengkapan unsur isi prosiding (10%)	3,00		3,00
b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		8,00
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9,00		8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		8,50
Total = (100%)	30,00		27,50
Nilai Pengusul = (60% x 27,5) = 16,5			

Catatan Penilaian Paper oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi paper:** Kelengkapan unsur isi jurnal telah terpenuhi karena pada artikel tersebut terdapat judul, abstrak, pendahuluan, metode, hasil dan pembahasan, kesimpulan dan referensi. Daftar referensi pada artikel sebanyak 23 literatur bereputasi.
- Ruang lingkup dan kedalaman pembahasan:** Dalam artikel ini penulis dapat memprediksi peningkatan porositas pada persimpangan antar sel dengan mengamati interaksi antara E-cadherin dan peptida ADTC. Informasi yang diperoleh dalam artikel ini berupa prediksi konformasi siklik ADTC7, energi ikatan, dan situs aktif pada peptida siklik ADTC7. Penulis dapat menunjukkan konformasi linear dan peptida siklik dan linear ADTC7.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** metodologi molecular docking dan molecular dynamic yang digunakan sangat mendukung dalam memperoleh informasi penting dalam artikel ini. Informasi yang terdapat dalam artikel sudah cukup lengkap yang didukung oleh referensi jurnal internasional bereputasi. 34 % referensi terbit 5 tahun sebelum artikel ini terbit.
- Kelengkapan unsur dan kualitas terbitan:** Artikel ini sudah memenuhi kualitas terbitan karena diterbitkan oleh IOP Publishing merupakan salah satu penerbit prosiding konferensi terbesar di dunia, yang menyediakan proses publikasi yang cepat, mudah digunakan, dan efektif bagi penyelenggara dan penulis.

Semarang, 9 April 2023
 Reviewer 2



Prof. Dr. Meiny Suzery, MS
 NIP. 196005101989032001
 Unit Kerja : Kimia FSM Undip

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b. Ruang lingkup dan kedalaman pembahasan (30%)	9,00		8,00
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	9,00		8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00		9,00
Total = (100%)	30,00		28,00
Nilai Pengusul = (60% x 28,00) = 16,8			

Catatan Penilaian Paper oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi paper:** Setiap bab dalam artikel saling terkait satu sama lain dengan penjelasan yang cukup jelas, sesuai dengan kaidah penulisan ilmiah yang baik dan benar. Unsur jurnal sudah lengkap, meliputi; Judul, Abstrak, Pendahuluan, Metode, Hasil dan Pembahasan, Kesimpulan, dan Referensi. Daftar referensi sebanyak 23 literatur yang sudah bereputasi. (3)
- Ruang lingkup dan kedalaman pembahasan:** Penulis membahas tentang interaksi pada jalur paraseluler yang terjadi pada peptida siklik ADTC7 yang mempengaruhi porositas pada interaksi EC1-EC2, sehingga obat-obatan dapat spesifik menuju otak. Cakupan yang dibahas berupa; konformasi terbaik dari siklik ADTC7, energi pengikatan, dan parameter sisi aktif dengan metode docking. Penulis dapat menjabarkan kemungkinan-kemungkinan konformasi molekul, sehingga hasil yang diperoleh merupakan hasil terbaik dari banyak kemungkinan. Penulis juga mendapat informasi perubahan yang terjadi antara ligan dan reseptor yang terjadi pada interaksi ADTC7 dengan EC1-EC2 dan memperoleh konformasi terbaiknya. Metode perlu ditingkatkan untuk menambah kedalaman pembahasan mengenai energi HOMO-LUMO sebagai parameter lain dalam penentuan konformasi terbaik dari ADTC7. Tabel 3 tidak dibahas serta tabel 6 tidak disitasi (8)
- Kecukupan dan kemutakhiran data/informasi dan metodologi:** Informasi serta data yang ditampilkan dalam artikel ini sudah cukup untuk kajian kimia komputasi dengan dilengkapi dasar referensi jurnal internasional bereputasi. 34 % referensi yang disitasi adalah terbit 5 tahun ke bawah, namun ada ref yang tertulis tanpa tahun (8)
- Kelengkapan unsur dan kualitas terbitan:** IOP Publishing adalah perusahaan penerbitan Institute of Physics. Penerbit tersebut menyediakan publikasi melalui mana penelitian ilmiah didistribusikan di seluruh dunia, termasuk jurnal, situs web komunitas, majalah, proses konferensi dan buku. Pada artikel ini berupa terbitan prosiding oleh IOP Publishing yang sudah berindeks scopus dengan nilai SJR 0,2 (2019). (9)
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Reviewer 1

A handwritten signature in black ink, consisting of a stylized 'M' followed by a cursive 'C' and 'D'.

Prof. Dr. Muhammad Cholid Djunaidi, S.Si., M.Si
NIP 19700702 199603 1 004
Unit Kerja : Kimia FSM Undip

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Komponen Yang Dinilai	Nilai Reviewer		Nilai Rata-rata
	Reviewer I	Reviewer II	
a. Kelengkapan unsur isi prosiding (10%)	3,00	3,00	3
b. Ruang lingkup dan kedalaman pembahasan (30%)	8,00	8,00	8,00
c. Kecukupan dan kemutakhiran data/informasi dan metodologi (30%)	8,00	8,00	8,00
d. Kelengkapan unsur dan kualitas terbitan/prosiding(30%)	9,00	8,50	8,75
Total = (100%)	28,00	27,50	27,75
Nilai Pengusul = (60% x 27,75) = 16,65			

Semarang, 9 April 2023

Reviewer 2



Prof. Dr. Meiny Suzery, MS
NIP. 196005101989032001
Unit Kerja : Kimia FSM Undip

Reviewer 1



Prof. Dr. Muhammad Cholid Djunaedi, S.Si., M.Si
NIP 19700702 199603 1 004
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Probing the interaction between EC1-EC2 domain of E-cadherin with conformational structure of cyclic ADTC7 (Ac-CDTPDC-NH₂) peptide using molecular docking approach

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^a Physical Chemistry Laboratory, Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia

^b Biochemistry Laboratory, Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia

^c Faculty of Biotechnology, Atma Jaya Catholic University of Indonesia, Jakarta, Indonesia

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Aisyafalah, S. , Hudiyanti, D. , Asy'Ari, M.
(2021) *Journal of Physics: Conference Series*

The validation of molecular interaction among dimer chitosan with urea and creatinine using density functional theory: In application for hemodialysis membrane

Siahaan, P. , Sasongko, N.A. , Lusiana, R.A.
(2021) *International Journal of Biological Macromolecules*

Computational study: Noncovalent interaction of cys-ala peptide with alkaline earth metal ions and its conformation changes

Tresnoningtias, M.A. , Nurwarrohman, A.S. , Ihyar, K.
(2021) *Key Engineering Materials*

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Fine-tuning the physicochemical properties of peptide-based blood-brain barrier shuttles

Ghasemy, S. , García-Pindado, J. , Aboutaleb, F.
(2018) *Bioorganic and Medicinal Chemistry*

Shuttle-mediated drug delivery to the brain

Malakoutikhah, M. , Teixidó, M. , Giral, E.
(2011) *Angewandte Chemie - International Edition*

MiniAp-4: A Venom-Inspired Peptidomimetic for Brain Delivery

Oller-Salvia, B. , Sánchez-Navarro, M. , Ciudad, S.

Abstract

Increasing significantly brain disease every year make difficult to help people who suffer disease in their brain. Drug delivery can be reached through a paracellular pathway. The use of the derivative cadherin peptides (ADT and HAV) to enhance the porosity in this pathway was investigated. The aim of this studied to determine the best conformation of cyclic ADTC7 peptide which interacts with EC1-EC2 domain of E-cadherin with energy binding and active sites parameters. The methods used in this study are: 1). MD simulation using GROMACS software, and 2). Molecular docking with AutoDock software. The variation used on MD simulation are atomic distances and constant restrains in atom S14...S78 for 20 ns. The result of MD simulation for 20 ns shows that the linear and cyclic ADTC7 peptide are -118,824.84 kJ.mol⁻¹ and -52,985.95 kJ.mol⁻¹, respectively. The best conformation of cyclic ADTC7 peptide with the EC1-EC2 domain of E-cadherin is C1 with the lowest binding energy of -24.56 kJmol⁻¹. The active site at residues such as Val3, Ile4, Pro5, Pro6, Ile7, Ser8, Leu21, Val22, Gln23, Lys25. It has RMSD value less than 2 Å, low energy binding and low inhibition constant, a large population and a stable pose when validation docking. © Published under licence by IOP Publishing Ltd.

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🔗 Siahaan, P.; Physical Chemistry Laboratory, Department of Chemistry, Faculty of Sciences and Mathematics, Diponegoro University, Semarang, Indonesia; email:siahaan_parsaoran@yahoo.com
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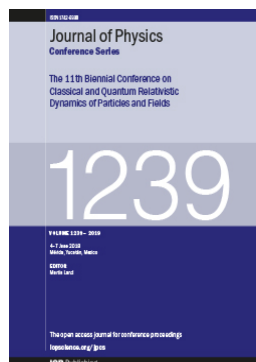
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The 9th iSNPiNSA

LIST OF SPEAKER

I. Keynote Speaker

No.	Name	Research Field	Institution	Country
1.	Prof. Emmanuel Cornillot	Biotechnology	Universite de' Montpellier	Perancis
2.	Prof. Dr. Baba Musta	Geochemistry	Faculty of Science, UMS	Malaysia
3.	Prof. Dr. Ir. Rokhmin Dahuri, MS.	Marine Resource and Environmental Studies	President of Indonesian Aquaculture Society; Proffesor in Marine Resource and Environmental Studies	Indonesia
4.	Sapto P. Putro, M.Si., Ph.D.	Marine Ecology and Aquaculture	Faculty of Science and Mathematics, Diponegoro University	Indonesia

II. Invited Speaker

No.	Name	Department	Institution	Country
1.	Dinar Mutiara Kusumo Nugraheni, S.T., M.InfoTech.(Comp).	Computer Science	FSM UNDIP	Indonesia
2.	Dr. Eng. Ali Khumaeni, S.Si., MS	Physics	FSM UNDIP	Indonesia
3.	Dr. M. Cholid Djunaidi, M.Si.	Chemistry	FSM UNDIP	Indonesia
4.	Dr. Lilih Khotimperwati, S.Si., M.Si.	Biology	FSM UNDIP	Indonesia
5.	Dr. Tarno, M.Si.	Chemistry	FSM UNDIP	Indonesia
6.	Farikhin, M.Sc. Ph.D.	Mathematics	FSM UNDIP	Indonesia

D. Conference Organizers

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Dr. Kusworo Adi, S.Si., MT. (Steering Committee)
Drs. Sapto P. Putro, M.Si., Ph.D (Steering Committee)
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Table of contents

Volume 1524

2020

◀ Previous issue Next issue ▶

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Interaction between madden-julian oscillation and monsoon related to big floods over south sulawesi in january 2019

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Cleaner sheep leather tanning process using *uncaria gambir*: the influence of rebating on leather properties

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Horizontal gradient analysis of gravity data for subsurface fluid flow identification (case study: cilincing, north jakarta)

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Measurement of eye lens doses estimation in interventional radiology

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Study of low head turbine propellers axial flow for use of micro-hydropower plant (MHP) in Aceh, Indonesia

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Database replication method for real-time measurement pH parameter of fishery using a wireless sensor system

W H Sugiharto, M I Ghazali, H Susanto, M A Budihardjo and S Suryono

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Development of electrooptic devices by strengthening electromagnetic fields using colloidal silver solutions

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Synthesis of gadolinium nanoparticles in spinach-extracted liquid using a pulse laser ablation method

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Effects of repetition rate on the identification of elements in gemstone using the LIBS method

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Analysis of signal to noise ratio from 1.5 tesla MRI head coil phantom image on daily quality assurance

G Maslebu, E S D Kusriani and A Setiawan

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Fabrication and properties of high efficiency dye-sensitized solar cells (DSSCs) with photon absorption optimization

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Characterization of the radiosensitization effect of pulsed laser ablated-gadolinium

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Low-temperature process for green tea drying using zeolite adsorption integrated fluidized bed dryer

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Energy and exergy analysis economic of continuous vibrating fluidized bed drying on celery dryingS U Handayani, I S Ariananto, P T Purno and S Pujawara
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Growth of collagen-nanosilver (Co-AgNP) biocomposite film with electrospinning method for wound healing applications

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Construction of lyapunov function using gradient method to stability analysis of the nitrogen-phosphate-phytoplankton-sediment interaction model

Widowati, S P Putro and E Triyana

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K-nearest neighbor (KNN) with global GINI diversity index for classification subsidy food in Semarang city, Indonesia

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Hoax news validation using similarity algorithms

S Y Yuliani, S Sahib, M F Abdollah, Y S Wijaya and N H M Yusoff

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3D modeling of subsurface jiwo fault around gantiwarno sub-district, klaten district, central java using the magnetic method

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The first fundamental group of Kronecker quaternion group

A Adrianda and Y Yanita

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Village classification index prediction using geographically weighted panel regression

A S Ningrum, A Rusgiyono and A Prahutama

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Efficiency nonminimally supported design for three parameters weighted exponential model

T Widiharih, M A Mukid and Mustafid

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Γ – semigroup generated by a semigroup

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The algebraic structure on the neutrosophic triplet set

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WAC4 algorithm to solve the multiperiod degree constrained minimum spanning tree problem

Wamiliana, A Junaidi, Amanto, M Usman and Warsono

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Counting the number of vertexes labeled connected graphs of order five with minimum five edges and maximum ten parallel edges

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012048

Comparison of performance of k-nearest neighbor algorithm using smote and k-nearest neighbor algorithm without smote in diagnosis of diabetes disease in balanced data

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Analysis of variance for strip plot design with missing values: bias correction of the mean squares

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Stability analysis of mathematical model (*sirb*) in the spread of cholera with vaccination and disinfection

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Secondary metabolites in *elaecarpus grandiflorus* cell culture in WPM medium with various concentrations of PGR

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The impact of mangrove plantation in ponds on the secondary metabolite content

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Analysis total plate count (tpc) and organoleptic test on seaweed chips

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Characterization of citronella grass essential oil of *Cymbopogon winterianus* from Batang region, Indonesia

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Histologic response of aortic *Rattus norvegicus* male strain wistar hyperlipidemia after giving kersen fruits juice and extract lakum leaves

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Isolation and identification of rare actinomycete-like bacteria from soil-based on 16S ribosomal RNA gene sequences

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The potential of mixed epibiotic (binahong leaves, *anrederacordifolia*, and garlic, *allium sativum*, extracts) as a feed additive to combat *aeromonashydrophilain* infection on catfish (*clariasgariepinus*)

Sarjito, S B Prayitno, N T Kusuma and Desrina

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The density of microplastic in sea cucumber (*Holothuria* sp.) and sediment at Tidung Besar and Bira Besar island, Jakarta

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Production of coco-vinegar in a bubble biofermentor

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Antibacterial activity tests of isolate endophytic bacteria from the tea plant (*Camellia sinensis*) againsts *Staphylococcus aureus* and *Staphylococcus epidermidis*

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The control system for the nutrition concentration of hydroponic using web server

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Leaf anatomy response of several varieties of rice (*Oryza sativa* L.) to the application of silica fertilizers

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Preparation and characterization of lignin nanoparticles from rice straw after biosynthesis using *Lactobacillus bulgaricus*

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Bioethanol production using the SSF method (*simultaneous saccharification and fermentation*) of microalgae *anabaena* sp.

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Probing the interaction between EC1-EC2 domain of E-cadherin with conformational structure of cyclic ADTC7 (Ac-CDTPDC-NH₂) peptide using molecular docking approach

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Purwoceng chemical characterization by FTIR spectrum and feasibility analysis of jelly purwoceng diversification with the addition of gelatine and carrageenan

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Case study of malaria patients: distribution of cases and maps of *Anopheles sp.* breeding place in Kaligesing sub-district, Purworejo district

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Dynamical analysis model of HIV-1 infection in CD4⁺ T cells with antibody response

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Classification of liver cancer with microrna data using the deep neural network (DNN) method

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Oil content analysis on yam bean fermented by *Aspergillus niger*

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The growth and potential of *gamma-aminobutyric acid* (GABA) by lactic acid bacteria isolated from fish fermented food from Maluku, Indonesia

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Study on water quality physical-chemical parameters aquaculture areas in Menjangan Besar Island, Kepulauan Karimunjawa, Jepara, Indonesia

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Nutritive and antioxidative properties of some selected agro-industrial by-products fermented with the fungus *Chrysonillia crassa* as alternative feedstuffs for poultry

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Subsurface mapping of University Diponegoro Tembalang campus based on resistivity data

A Setyawan, R Gernowo, E S Jatmiko, Wijayaningrum, Y Aribowo and Najib

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Isolation and identification of rare actinomycete-like bacteria from soil-based on 16S ribosomal RNA gene sequences

Y Eshananda¹, F Ningsih^{1,2}, Y Sakai^{3,4}, A Yokota³, S Yabe^{3,4}, W Sjamsuridzal^{1,2}

¹Department of Biology, Faculty of Mathematics and Natural Sciences, Universitas Indonesia, Kampus UI Depok, Depok 16424, Indonesia

²Center of Excellence for Indigenous Biological Resources-Genome Studies, Faculty of Mathematics and Natural Sciences, Universitas Indonesia, Kampus UI Depok, Depok 16424, Indonesia

³Department of Microbial Resources, Graduate School of Agricultural Science, Faculty of Agricultural, Tohoku University, 468-1 Aoba, Aramaki, Sendai, Miyagi 980-0845, Japan

⁴Hazaka Plant Research Center, Kennan Eisei Kogyo Co., Ltd., 44 Aza-Inariyama, Oaza-Ashitate, Murata-Cho, Shibata gun, Miyagi 989-1311, Japan.

Corresponding author: yuriza.eshananda@ui.ac.id

Abstract. The rare actinomycete-like bacteria are mycelium-forming bacteria other than phylum *Actinobacteria* that difficult to isolate and cultivate. This group of bacteria was recently speculated by many scientists as a potential new microbial resource for the discovery of novel compounds, as a substitute for actinomycetes. In this study, we isolate and identify rare actinomycete-like bacteria from forest soil collected under bamboo trees, near the CisolokGeysers, Sukabumi, Indonesia. The isolation of bacteria was performed using Reasoner's 2A (1:10 dilution) medium with 2% gellan gum instead of agar and incubated at 30 °C for three weeks. The 16S rRNA gene sequences of the isolates were examined to determine their taxonomic position. Four isolates designated K17-1, K17-2, K42, and K44 showed pale oranges colonies and formed mycelia were obtained. The results of 16S rRNA gene sequences of these isolates showed high similarity to members of the genus *Dictyobacter* in the family *Dictyobacteraceae* of the class *Ktedonobacteria* of the phylum *Chloroflexi*, with values 97.16-98.02%, and most closely related to the species *Dictyobacteraurantiacus* S-27^T (97.16-98.02% similarities). This result suggested that the member of the class *Ktedonobacteria*, which considered as rare actinomycete-like bacteria, such as *Dictyobacter* could be found in the forest soil of the geothermal area.

1. Introduction

Actinobacteria are gram-positive bacteria that have a high percentage of guanine and cytosine in their genome [1]. This group morphologically comprises unicellular organisms to mycelium-forming bacteria which called Actinomycetes [1,2]. However, bacteria that have filamentous appearance also could be found in the phylum *Chloroflexi*. The member of this phylum which has actinomycete-like morphology is present in the four different class namely *Chloroflexi*, *Anaerolineae*, *Caldilineae* and *Ktedonobacteria* [3]. Among these class, *Ktedonobacteria* has some obvious morphological features which distinguish themselves from others. The member of *Ktedonobacteria* are aerobic organism and forming branched mycelia with spores like actinomycetes [3,4]. Moreover, most validly published strains of *Ktedonobacteria* budding their multiple spores per cell on the aerial mycelium which unique among bacteria [5]. All of *Ktedonobacteria* identified as gram-positive bacteria while almost of the member in phylum *Chloroflexi* were gram-negative [3,6]. Based on these exceptional characters, class *Ktedonobacteria* could be included as the rare actinomycete-like bacteria.

Rare actinomycete-like bacteria could provide an alternative for the discovery of new compounds derived from microorganisms because spore formation usually would be followed by the production of secondary metabolites [7,8]. Further analysis of the genomic of nine members of rare actinomycete-like bacteria



Hoax news validation using similarity algorithms

S Y Yuliani^{1,2}, S Sahib², M F Abdollah², Y S Wijaya, N H M Yusoff

¹Information Security and Networking Research Group (InFORSNET), Faculty of Information Communication Technology, Universiti Teknikal Malaysia Melaka Malaka, **Malaysia**

²Informatic Department, Faculty Engineering, University Widyatama Bandung, Indonesia

Corresponding author: sy.yuliany@gmail.com

Abstract. News that is presented every day on social media dramatically affects the feelings, feelings, thoughts, or even actions of a person or group. Hoax News is one of them which is disturbing the public and raising noise in various fields, ranging from politics, culture, security, and order, to the economy. Inseparable from social media users. How every day, there is information on social media, which is not necessarily true so that people are provoked by hoax on social media. The news detection system in this study was designed using Unsupported Learning so that it does not require data training. The system was built using the Equation algorithm to calculate the validity of document similarity. Extraction results used to search for content related to user input using a detection engine, then the similarity value and the time needed to utilize hoax news are calculated. System validation testing by using a four text similarity algorithm called the Equation algorithm, the Levenshtein algorithm, the Smith-Waterman algorithm, the Damerau Levenshtein algorithm; this algorithm is used to find the best analytical solution of news hoaxes and submissions needed to find the news hoax password. The final results of the deception detection research using a script that has been done for Validation using an algorithm, get the value of accuracy in detection using the Smith-Waterman algorithm, which produces an accuracy value of text similarity of 99.29% and can be used a process of 6, 57 seconds, followed by the second sequence that is the similarity algorithm produces an accuracy of 75% and requires a processing time of 4.94 seconds, then the third sequence is the Levenshtein algorithm with an accuracy of 55.02% and requires a processing time of 5.49 seconds, and is used today is Damerau Levenshtein algorithm is 55.02% and requires a processing time of 7.54%. The results of research tests on this text can conclude the more text on the detection engine, the higher the verification value and the higher the time needed to process hoax news.

1. Introduction

Sharing information is a positive thing, but not all information disseminated through social media is in the form of facts. There have been various cases of spreading the news that is not facts or often called hoaxes. Whereas hoax is critical information that misleads human perception by spreading false information but considered as valid, No wonder then the intensity of fake news and hoax news on social media is so viral on social media [1]. For personal and group benefit by spreading harmful content that caused unrest and mutual suspicion in the community [2]. The ease and speed of dissemination on social media make this hoax news known to many people in a relatively short period, and can to more people.



Subsurface mapping of University Diponegoro Tembalang campus based on resistivity data

A Setyawan¹, R Gernowo¹, E S Jatmiko¹, Wijayaningrum², Y Aribowo³, Najib³

¹Department of Physics, Faculty of Science and Mathematics, Universitas Diponegoro, Jl. Prof. Soedharto, SH, Tembalang, Semarang 50275, **Indonesia**

² Undergraduate Student Department of Physics, Faculty of Science and Mathematics, Universitas Diponegoro, Jl. Prof. Soedharto, SH, Tembalang, Semarang 50275, Indonesia

³Department of Physics, Faculty of Science and Mathematics, Universitas Diponegoro, Jl. Prof. Soedharto, SH, Tembalang, Semarang 50275, Indonesia

Corresponding author: agussetyawan@fisika.fsm.undip.ac.id

Abstract. Subsurface mapping using the geoelectric method has been carried out in the area of Undip Campus, Tembalang to determine the distribution of subsurface layers resistivity. This study employs the Wenner configuration geoelectric method. Data were collected at seven points with a track length of 100 meters and a distance among electrodes of 5 meters. Data processing is carried out using RES2DINV software packages that produce rock resistivity values and depth estimates, then the interpretation of each track is carried out in detail by taking into account the geological information available in the Undip campus, Tembalang. The results of the interpretation show that the study area is dominated by breccias which are Kaligetas formations. The breccia rocks themselves are claystone which tends to be water-resistant and there is also sandstone. Nearly every data collection point has the same cross-section. Claystone with resistivity ranges from 3.05 Ωm to 26.5 Ωm . Sandstones with resistivity range from 20.0 Ωm to 135 Ωm . The rest found alluvium and sand with a resistivity of almost more than 100 μm .

1. Introduction

Diponegoro University was located in Tembalang District, Semarang is one of the best public universities in Indonesia. Construction of infrastructure facilities on campus is continuously carried out to support the learning process and the progress of Diponegoro University. Development activities include the construction of: reservoirs, parking buildings, lecture buildings, sports facilities, irrigation, final disposal, etc. The development requires the preparation of land and carrying capacity of the region. Integrated mapping is needed not only on the surface but also on the subsurface is very important. So in this study, we focus on mapping the subsurface conditions based on the distribution of resistivity values using resistivity geoelectric method. The principle of resistivity geoelectrical method is injection the current through the subsurface to obtain the potential value of the rocks and to get resistance value [1][2][3]. Wenner configuration selection is preferred for mapping with shallow depth. Furthermore, Sudarsono 1984, revealed the need to study the characteristics of the land and its functions so that they could predict what to do when loading occurred on the land.

The results of the mapping are expected to provide information about soil conditions including soil layers, soil structure, soil conditions, bedrock depth, stability. The information obtained will be used as a reference for the next infrastructure work.

