**LEMBAR**
**HASIL PENILAIAN SEJAWAT SEBIDANG ATAU *PEER REVIEW***
**KARYA ILMIAH: PROSIDING**

| | | |
|---|---|---|
| Judul Publikasi Ilmiah (Artikel) | | : Probing the Interaction between Cyclic ADTC1 Ac-CADTPPVC-NH2) Peptide with EC1-EC2 domain of E-cadherin using Molecular Docking Approach |
| Jumlah Penulis | | : 5 orang |
| Status Pengusul | | : penulis anggota |
| Identitas Jurnal Ilmiah | a. Nama Jurnal Ilmiah: | : IOP Conference Series: Materials Science and Engineering |
| | b. Nomor ISBN /ISSN | : ISSN: 17578981 |
| | c. Volume, Nomor, Bulan, Tahun | : Volume 349, Issue 1, 2 May 2018, Article number 012050 |
| | d. Penerbit | :IOP Publishing |
| | e. DOI artikel (jika ada) | https://doi.org/10.1088/1757-899X/349/1/012050 |
| | f. Alamat web jurnal | http://iopscience.iop.org/issue/1757-899X/349/1 |
| | g. Terindeks di SCOPUS (CiteScore is 0.53), Scimago journal Rank (**H-index 24, SJR 0.19**), Google Scholar, dll | |
| | e. Jumlah Halaman | :8 (1-8) halaman |

Kategori Publikasi Jurnal Ilmiah : √ ~~Jurnal Ilmiah Internasional~~ / **Internasional Bereputasi (prosiding)****
☐ Jurnal Ilmiah Nasional Terakreditasi
☐ Jurnal Ilmiah Nasional/Nasional Terindeks di DOAJ, CABI, COPERNICUS**

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| b. Ruang lingkup dan kedalaman pembahasan (30%) | 7 | 9 | 8 |
| c. Kecukupan dan kemutahiran data/informasi dan metodologi (30%) | 8 | 8,1 | 8,05 |
| d. Kelengkapan unsur dan kualitas penerbit (30%) | 8 | 9 | 8,5 |
| **Total = (100%)** | 26 | 29,1 | 27,55 |
| **Nilai Pengusul = (40% x total)/4 =** | 2,6 | 2,91 | 2,755 |

Semarang,

Reviewer 2

Prof. Dr. rer. nat Nuryono, M.S.
NIP. 196407141988111001

Unit kerja : Universitas Gadjah Mada Yogyakarta
Jabatan Fungsional : Guru Besar
Bidang ilmu : Kimia

Reviewer 1

Prof. Dr. Moh Djaeni, ST, M.Eng
NIP 197102071995121001

Unit Kerja : Universitas Diponegoro Semarang
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

**LEMBAR**
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**KARYA ILMIAH: PROSIDING**

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| | f. Alamat web jurnal | http://iopscience.iop.org/issue/1757-899X/349/1 |
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☐ Jurnal Ilmiah Nasional Terakreditasi
☐ Jurnal Ilmiah Nasional/Nasional Terindeks di DOAJ, CABI, COPERNICUS**

~~Hasil Penilaian~~ *Peer Review*

| Komponen Yang Dinilai | Nilai Maksimal Jurnal Ilmiah | | | Nilai Akhir yang diperoleh |
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| | Internasional Bereputasi Berimpact factor (prosiding) | Nasional Terakreditasi | Nasional | |
| | (30) | | | |
| a. Kelengkapan unsur isi prosiding (10%) | 3 | | | 3 |
| b. Ruang lingkup dan kedalaman pembahasan (30%) | 9 | | | 7 |
| c. Kecukupan dan kemutahiran data/ informasi dan metodologi (30%) | 9 | | | 8 |
| d. Kelengkapan unsur dan kualitas penerbit (30%) | 9 | | | 8 |
| **Total = (100 %)** | 30 | | | 26 |
| **Nilai Pengusul = (40% x 26)/4 = 2.6** | | | | 2.6 |

**Catatan Penilaian artikel oleh Reviewer :**

1. **Kesesuaian dan kelengkapan unsur isi artikel:**
   Artikel sangat lengkap, dimana analisis tentang interaksi antara cyclic adtc1 ac-cadtppvc-nh2) peptide dengan domain ec1-ec2 dari e-cadherin menggunakan pendekatan docking molekul disajikan dengan terperinci, disitasi dan dibahas. Topik dan materi sesuai dengan jurnal yang bersangkutan. Tata penulisan tersaji dengan sangat baik.
2. **Ruang lingkup dan kedalaman pembahasan:**
   Artikel ini membahas tentang interaksi antara cyclic adtc1 ac-cadtppvc-nh2) peptide dengan domain ec1-ec2 dari e-cadherin menggunakan pendekatan docking molekul. Tujuan dari penelitian ini adalah untuk menyelidiki efek alanine asam amino (A) dari ADTC1 pada sifat interaksinya. Hasil penelitian menunjukkan bahwa CC dari kotak F ADTC1 memiliki interaksi terbaik dengan energi ikat -26,36 kJ / mol dan energinya lebih rendah dari ADTC5 tanpa asam amino alanin. ADTC1 berinteraksi dengan EC1 dari EC1-EC2 di Asp1, Trp2, Val3, Ile4, Ile24, Lys25, Ser26, Asn27, dan Residu met92. Pembahasan dan hasil yang ditampilkan terlalu singkat.
3. **Kecukupan dan kemutakhiran data/informasi dan metodologi:**
   Referensi yang dicitasi dalam artikel ini ada **15** dimana **10** Baru (dalam 10 tahun terakhir). Nilai novelty/kebaruan artikel cukup baik. Metode disajikan dengan tahapan yang jelas, dan mudah diikuti.
4. **Kelengkapan unsur dan kualitas terbitan:**
   Penerbit adalah IOP Publishing dan terindeks Scopus, SJR 0.19, H-index 24. Nilai similaritas artikel berdasarkan Turnitin hanya 2%, sehingga orisinalitas sangat baik.

Semarang, November 2019
Reviewer

Prof. Dr. Moh Djaeni, ST, M.Eng
NIP 197102071995121001
Unit Kerja : Universitas Diponegoro
Jabatan Fungsional : Guru Besar
Bidang Ilmu : Teknik Kimia

**LEMBAR**
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Kategori Publikasi Jurnal Ilmiah : √ ~~Jurnal Ilmiah Internasional~~ / **Internasional Bereputasi (prosiding)****
□ Jurnal Ilmiah Nasional Terakreditasi
□ Jurnal Ilmiah Nasional/Nasional Terindeks di DOAJ, CABI, COPERNICUS**

Hasil Penilaian *Peer Review*

| Komponen Yang Dinilai | Nilai Maksimal Jurnal Ilmiah | | | Nilai Akhir yang diperoleh |
|---|---|---|---|---|
| | Internasional Bereputasi Berimpact factor (prosiding) | Nasional Terakreditasi | Nasional | |
| | (30) | | | |
| a. Kelengkapan unsur isi prosiding (10%) | 3 | | | 3 |
| b. Ruang lingkup dan kedalaman pembahasan (30%) | 9 | | | 9 |
| c. Kecukupan dan kemutahiran data/ informasi dan metodologi (30%) | 9 | | | 8,1 |
| d. Kelengkapan unsur dan kualitas penerbit (30%) | 9 | | | 9 |
| **Total = (100 %)** | 30 | | | |
| **Nilai Pengusul = (40% x 29,1)/4 = 2,91** | | | | 29,1 |

**Catatan Penilaian artikel oleh Reviewer :**

a. **Kesesuaian dan kelengkapan unsur isi Jurnal:**
Proseding diterbitkan dalam IOP Conference Series: Materials Science and Engineering. Artikel yang diterbitkan mengandung unsur-unsur sangat lengkap. Artikel dalam proseding ini membahas interaksi antara cyclic adtc1 ac-cadtppvc-nh2) peptide dengan domain ec1-ec2 dari e-cadherin menggunakan pendekatan docking molekul. Similaritas artikel berdasarkan Turnitin hanya 2% (tingkat orisinalitas sangat baik).

b. **Ruang lingkup dan kedalaman pembahasan:**
Runag lingkup artikel iniadalah interaksi antara cyclic adtc1 ac-cadtppvc-nh2) peptide dengan domain ec1-ec2 dari e-cadherin menggunakan pendekatan docking molekul, yang cukup dan layak untuk dipublikasikan dalam proseding. Kedalaman pembahasan cukup mendalam dan detail, didukung dengan referensi dari jurnal.

c. **Kecukupan dan kemutakhiran data/informasi dan metodologi:**
Data penelitian yang disajikan cukup dan layak untuk di proseding. Kemutakhiran informasi tinggi, yang ditunjukkan oleh referensi sebanyak **15, 10** (67%) terbit dalam 10 tahun terakhir. Kebaruan artikel tinggi. Metode dan prosedur penelitian secara komptasi kimia disajikan dengan tahapan yang jelas.

d. **Kelengkapan unsur dan kualitas Penerbit:**
Penerbit proseding ini adalah IOP Publishing yang telah terindeks Scopus, SJR 0.19, H-index 24.

Yogyakarta, November 2019
Reviewer

Prof. Dr. rer. nat Nuryono, M.S.
NIP. 196407141988111001
Bidang ilmu/Unit kerja :
Departemen Kimia pada Fakultas MIPA UGM Yogyakarta

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IOP Conference Series: Materials Science and Engineering
Volume 349, Issue 1, 2 May 2018, Article number 012050
12th Joint Conference on Chemistry, JCC 2017; Crystall Ballroom, Aston Hotel and Convention CentreSemarang; Indonesia; 19 September 2017 through 20 September 2017; Code 136611

## Probing the Interaction between Cyclic ADTC1 Ac-CADTPPVC-$NH_2$) Peptide with EC1-EC2 domain of E-cadherin using Molecular Docking Approach

(Conference Paper) (Open Access)

Siahaan, P.[a] ✉, Wuning, S.[a] ✉, Manna, A.[a], Prasasty, V.D.[b], Hudiyanti, D.[a]

Save all to author list

[a]Departement of Chemistry, Faculty of Science and Mathematics, Diponegoro University, Indonesia
[b]Faculty of Biotechnology, Atma Jaya Catholic University of Indonesia, Indonesia

## Abstract

View references (15)

Deeply understanding that intermolecular interaction between molecules on the paracellular pathway has given insight to its microscopic and macroscopic properties. In the paracellular pathway, synthetic cyclic ADTC1 (Ac-CADTPPVC-$NH_2$) peptide has been studied to modulate EC1-EC2 domain, computationally using molecular docking method. The aim of this research is to probe the effect of amino acid alanine (A) of ADTC1 on its interaction properties. The study carried out in two steps: 1. the optimization using GROMACS v4.6.5 program and; 2. Determination of the interaction properties using AutoDock 4.2 program. The interaction was done for A-J box, and the best position of the binding site and binding energy on the OC and CC ADTC1 peptides against the EC1-EC2 domain of E-cadherin was selected. The result showed that the CC of the F box ADTC1 has the best interaction with binding energy of - 26.36 kJ/mol and its energy was lower than ADTC5 without alanine amino acid. ADTC1 interacted with EC1 of EC1-EC2 on Asp1, Trp2, Val3, Ile4, Ile24, Lys25, Ser26, Asn27, and Met92 residues. 

## SciVal Topic Prominence

Topic: Cadherins | Adherens Junctions | Cells

Prominence percentile: 95.020

## Indexed keywords

Engineering controlled terms: Amino acids | Binding sites | Glycoproteins | Molecular modeling | Peptides

Engineering uncontrolled terms: Amino acid alanines | Best position | E-cadherins | Interaction properties | Intermolecular interactions | Microscopic and macroscopic properties | Molecular docking | Paracellular

Engineering main heading: Binding energy

## Funding details

| Funding sponsor | Funding number | Acronym |
|---|---|---|
| | 2013 | |

Funding text

Authors would thank Prof. Teruna J. Siahaan, Ph.D. (Phar-macy Department, University of Kansas, US), for the valuable direction and discussion of the cells and drug delivery systems. Thanks to Prof. Krzysztof Kuczera, Ph.D. (Chemistry Department, University of Kansas, US) for in depth discussion of a computational modeling. Last but not least, thanks to the Indonesian Directorate General of Higher Education, which has funded this research through the Research and Technology Funding scheme 2013.

**ISSN:** 17578981
**Source Type:** Conference Proceeding
**Original language:** English
**DOI:** 10.1088/1757-899X/349/1/012050
**Document Type:** Conference Paper
**Sponsors:**
**Publisher:** Institute of Physics Publishing

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Improving in vivo brain delivery of monoclonal antibody using novel cyclic peptides

Ulapane, K.R. , Kopec, B.M. , Siahaan, T.J.
*(2019) Pharmaceutics*

Ab-initio computational study of noncovalent interaction between peptide and alkaline metal ions on HF/6-31 G** level

Siahaan, P. , Christian, R. , Fauziah, A.N.
*(2018) AIP Conference Proceedings*

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# Source details

## IOP Conference Series: Materials Science and Engineering

Scopus coverage years: from 2009 to 2019

ISSN: 1757-8981 E-ISSN: 1757-899X

Subject area: Engineering: General Engineering | Materials Science: General Materials Science

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Updated monthly

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| Materials Science — General Materials Science | #305/438 | 30th |

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# IOP Conference Series: Materials Science and Engineering

| | |
|---|---|
| **Country** | United Kingdom - SIR Ranking of United Kingdom |
| **Subject Area and Category** | Engineering<br>Engineering (miscellaneous)<br><br>Materials Science<br>Materials Science (miscellaneous) |
| **Publisher** | |
| **Publication type** | Conferences and Proceedings |
| **ISSN** | 17578981, 1757899X |
| **Coverage** | 2009-ongoing |
| **Scope** | The open access IOP Conference Series provides a fast, versatile and cost-effective proceedings publication service for your conference. Key publishing subject areas include: physics, materials science, environmental science, bioscience, engineering, computational science and mathematics. |

24

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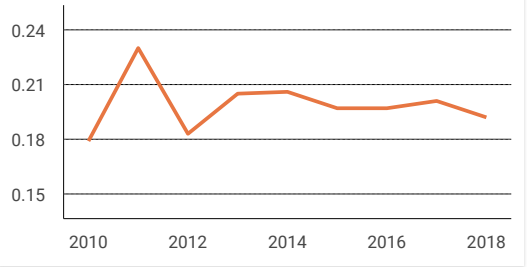


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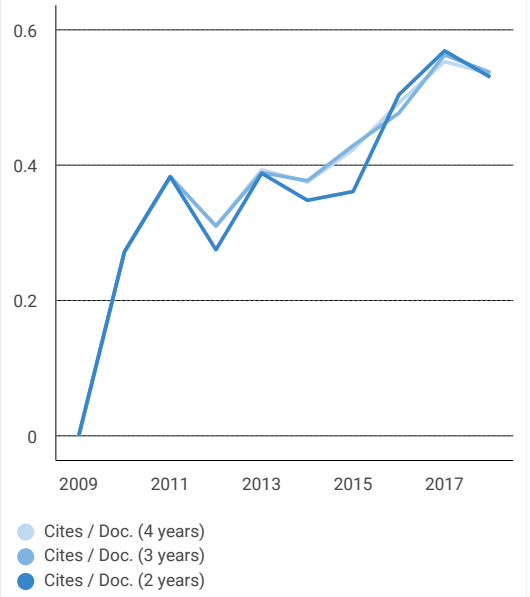


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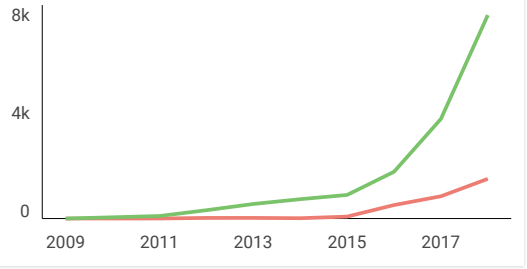


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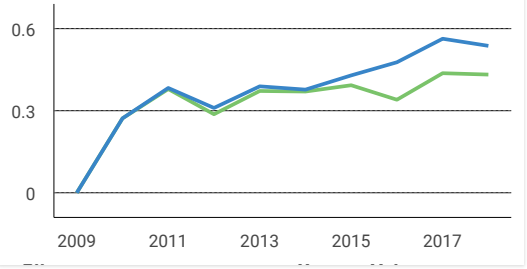
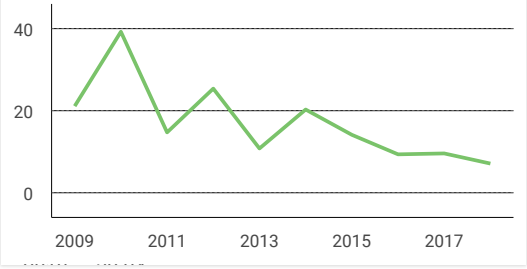



% International Collaboration

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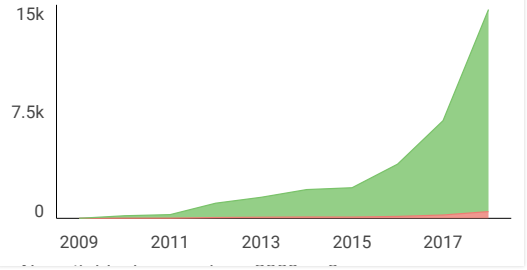


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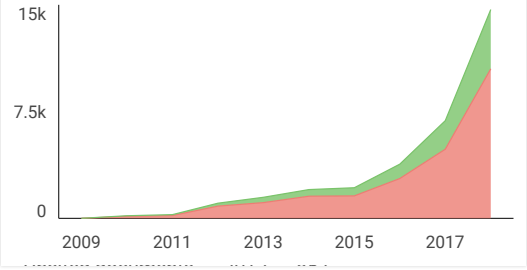



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# 12th Joint Conference on Chemistry

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## 18 September 2017

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|---|---|---|
| **18.30 – 21.00** | **Wecloming Dinner** | **Aston Hotel ballroom** |

## 19 September 2017

| | |
|---|---|
| 07.00-08.15 | Registration |
| 08.15-08.35 | Opening Ceremony |
| | Indonesia National Athem |
| | Welcoming Dance |
| 08.35-08.40 | Chairman speech<br>**Cepi Kurniawan, PhD** |
| 08.40-08.50 | Welcoming from the head of department |
| 08.50-09.00 | Welcoming speech and opening the conference by the Dean<br>**Prof. Dr. Zaenuri M., S.E, M.Si, Akt.** |
| 09.00-09.20 | Coffee Break |
| 09.20-10.00 | **Prof. Guoping Chen**<br>Hybrid Scaffolds of Biodegradable Polymers and Biomimetic Matrices for Tissue Engineering Applications |
| | Chair: Sri Kadarwati, PhD |
| 10.00-11.00 | **Prof. David Harding**<br>Designing Molecular Switches: A Molecular Magnetism Approach |
| | **Prof. Hadariah Bahron**<br>Imines and Metals: Marriage Made in Heavens |
| | Chair: M. Alauhdin, PhD |
| 11.00-12.00 | **Prof. Kasmadi Imam Kasmadi**<br>The Cultivation of Religious Characters in Chemical Science Learning |
| | **Prof. Subramaniam Ramanathan** |
| | Chair: Sri Kadarwati, PhD |
| 12.00-13.00 | Lunch Break |
| 13.00-14.00 | **Prof. Ni Nyoman Tri Puspaningsih**<br>Strengthening The Academic Network on Bioresource Technology Research towards Green Industry |
| | **Prof. Hajime Hirao**<br>Computationally Exploring Complex Molecular Systems |
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| JCC2017007 | Formulation and Antifungal Activity of Ointment Type of M/A From Ethanol Extract of White Plumeria Leaves (Plumeria alba L.) on Candida albicans | D R Ningsih, Zusfahair, D Kartika, M. Lianasari |
| JCC2017008 | Preparation and Physico-Chemical Properties of Gracilaria/PVA/GA/CNT-Based Hydrogel for Slow/Controlled Release Material | Hendrawan Hendrawan1, Fitri Khoerunnisa2 , FerinaIhsani Ekawati3 , Yaya Sonjaya4 |
| JCC2017010 | Dynamic adsorption of mixtures of Rhodamine B, Pb(II), Cu(II) and Zn(II) ions on composites chitosan-silica-polyethylene glycol membrane | F. Widhi Mahatmanti1*, W. D. P. Rengga2, E. Kusumastuti1, Nuryono3 |
| JCC2017014 | ZrO2/bamboo leaves ash (BLA) Catalyst in Biodiesel Conversion of Rice Bran Oil | Is Fatimah1, Ana Taushiyah1, FitriBadriatun Najah1, Ulil Azmi1 |
| JCC2017016 | Probing the Interaction Between Cyclic ADTC1 (Ac-CADTPPVC-NH2) Peptide with EC1-EC2 domain of E-cadherin using the Molecular Docking Method | Parsaoran Siahaan1, Sri Wuning1, Atiatul Manna1, VivitriDewi Prasasty2, Dwi Hudiyanti1 |
| JCC2017022 | Increasing character value and conservation behavior through integrated ethnoscience chemistry learning (a case study in the department of science universitas negeri semarang) | Sudarmin1, Woro Sumarni2, Agung Tri Prasetya3 |
| JCC2017025 | Synthesis and Characterization of Diranitidinecopper(II) Sulfate Dihydrate | H Syaima1, S B Rahardjo2, and I M Zein2 |
| JCC2017028 | Synthesis and Characterization of SrO/Zeolite Nanoparticle as CatalystalTransesterification Reaction of Used Cooking Oil | Widiarti Nuni1, UtamiNofita Sari1, F. Widhi Mahatmanti1 Harjito1, Cepi Kurniawan1, Didik Prasetyoko2, Suprapto2 |
| JCC2017036 | Development of Assessment Instruments to Measure Critical Thinking Skills | Woro Sumarni1, Kasmadi Imam Supardi2, Nuni Widiarti3 |
| JCC2017037 | Application of Sodium Ligno Sulphonate as Surfactant In Enhanced Oil Recovery and Its Feasibility Test for TPN 008 Oil | N I Prakoso1, Rochmadi2 and S Purwono2 |
| JCC2017061 | Treatment of Waste Lubricating Oil by Chemical and Adsorption Process Using Butanol and Kaolin | Riyanto1, Bayu Ramadhan1 and Deni Wiyanti1 |
| JCC2017062 | The Effect of Temperature and Time in The Manufacture of Gelatin Powder from Waste Fish Scales as A Source of Food Protein Towards National Food Security | Muhammad Afandi1, Faqihudin Mubarok1, Muhammad Farid Thahir1, Pratika Febrianti1, Tissasera Iseki1, Suherman S.T,M.T1 |
| JCC2017063 | Two Bisabolanes from Curcuma xanthorrhiza Rhizomes and Their Antibacterial Activity | Hartiwi Diastuti1, Yana Maolana Syah2, LiaDewi Juliawaty2, Marlia Singgih3 |

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|---|---|---|
| JCC2017165 | Effectiveness Study of Drinking Water Treatment In Indonesian Regulation of Health Minister Using Adsorbent Clays Appeal Andisol In Lariat Heavy Metal Cadmium (Cd) and Bacterial Pathogens | Dr. Pranoto, M.Sc1, Inayati, S.T., M.T, Ph.2 , Fathoni Firmansyah3 |
| JCC2017166 | Radical Scavenging Activity from Ethanolic Extract of Malvaceae Family's Flowers | AnifNur Artanti1, Niki Rahmadanny1, Fea Prihapsara1 |
| JCC2017167 | Golden Wattle (Acacia pycnantha) Flower: Is it Only Floral Emblem of Australia? | Rudi Hendra1,2, Paul Keller2 |
| JCC2017169 | Electrochemical Disinfection of Coliform and Escherichia Coli for Drinking Water Treatment By Electrolysis Method Using Carbon Electrode | Riyanto1, Wanda Rusma Agustiningsih1 |
| JCC2017172 | Prenylation of Pinostrobin and Antibacterial Activity Against Clinical Bacteria | Soerya Dewi Marliyana1,, Didin Mujahidin2 and Yana M Syah2 |
| JCC2017178 | Simple Approach in Understanding Interzeolite Transformations Using Ring Building Units | Dede Suhendar1,2, Buchari2, Rino R. Mukti2, Ismunandar2 |
| JCC2017179 | The Effect of Mangoosteen Extract (GraciniaMangostana L.) on Synthesis of Ag3PO4Photocatalyst | Mohammad Afif1, Alfa Marcorius1, Khusnul Afifah1, Siti Nurfiah1, Khanifudin Khanifudin2, Febiyanto Febiyanto2, Uyi Sulaeman1* |
| JCC2017185 | Transformation of Indonesian Natural Zeolite into Analcime Phase under Hydrothermal Condition | WitriWahyu Lestari1, DienNur Hasanah1, Riandy Putra1,2, RinoRakhmata Mukti3, and KhoirinaDwi Nugrahaningtyas1 |
| JCC2017188 | Synthesis and Characterization of SrO/Zeolite Nanoparticle as CatalystalTransesterification Reaction of Used Cooking Oil | Widiarti Nuni1, UtamiNofita Sari1, F. Widhi Mahatmanti1 Harjito1, Cepi Kurniawan1, Didik Prasetyoko2, Suprapto2 |
| JCC2017189 | Ar-Turmerone a Sesquiterpenoid from Curcuma Soloensis. Val (TemuGlenyeh) Rhizome Extract | Gesti Munasah1, M. Widyo Wartono1, FajarRakhman Wibowo1, SoeryaDewi Marliyana1 |
| JCC2017193 | Identification and Control of Unknown Impurity in TrimetazidineDihydrohcloride Tablet Formulation | Jefri1, Didik Harmoko1, Agustina Dian Puspitasari2, Joseph Sunder Raj Talpaneni1, Raymond R Tjandrawinata1,2,3 |
| JCC2017197 | Modifications of Deoxynojirimycin (DNJ) Compound as Î±-Glucosidase Inhibitor for the Dengue Fever Treatment | Usman Sumo Friend Tambunan, HanumArizaDeski, Moch. ArifinFardiansyahNasution |
| JCC2017198 | 5-Subtituted Isatin Derivatives: Synthesis and Anti-tubercular Activity Against Mycobacterium tuberculosis H37Rv | M. RizaGhulam Fahmi1, Laili Khumaidah1, TrividiatiKhusnul Ilmiah1, Arif Fadlan1,Mardi Santoso1 |
| JCC2017199 | Formulation of Antibacterial Liquid Soap from Nyamplung Seed Oil (Calophylluminophyllum L) with Addition of Curcuma heyneana and its Activity Test on Staphylococcus aureus | Senny Widyaningsih1, Moch.Chasani1, Hartiwi Diastuti1, Novayanti1 |

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|---|---|---|
| JCC2017203 | Chitosan as Natural Coagulant to Minimize Hg (II) Levels in Bone River Waters of Gorontalo Province | Astin Lukum1, Asda Rauf2, Jefrin Akume1, ArfianiRizki Paramata3 |
| JCC2017206 | Adsorption Kinetics of Sodium Lauryl Sulfate (SLS) and Hexadecyltrimetilammonium Bromide (HDTMABr) Surfactants on Activated Carbon | Arnelli1, Aditama WP1, Zul Fikriani1, Yayuk Astuti1 |
| JCC2017207 | The Effect of Cellulose Acetate Concentration from Coconut Nira on Ultrafiltration Membrane Characteristics | Eva Vaulina1, Senny Widyaningsih1, Dwi Kartika1, Mia Putri Romdoni1 |
| JCC2017212 | Supramolecular Assembly of Group 11 Phosphorescent Metal Complexes for Chemosensors of Alcohol Derivatives | Hendrik O. Lintang1,2,3, NurFatiha Ghazalli4,5, Leny Yuliati1,2,3 |
| JCC2017216 | Ab Initio Computational Study of –N-C and –O-C Bonding Formation : Functional Group Modification Reaction Based Chitosan | Parsaoran Siahaan1SitiNurMilatus Salimah1, Marta J. Sipangkar1, Dwi Hudiyanti1, M. Cholid Djunaidi1, Marlyn Dian Laksitorini2 |
| JCC2017222 | Development of Performance Assesment Instrument Based on Contextual Learning to Measure Students Laboratory Skill | EndangSusilaningsih, KhusnulKhotimah, Sri Nurhayati |
| JCC2017224 | FTIR and FT-Raman analysis of Bentonite Modified with 3-aminopropyltrimethoxysilane | E. Pramono1,3, C. L. Radiman1, D. Wahyuningrum2, W. Pratiwi1 |
| JCC2017226 | Chemical and Physical Composition and Mosquito Repellent Activity of Fractionation Active Component from Java Citronella Oil (Cymbopogonwinterianus) | Willy Tirza Eden1, Dante Alighiri1, Edy Cahyono2, Kasmadi Imam Supardi3, Nanik Wijayati2 |
| JCC2017228 | Removal of Cadmium from Wastewater by Adsorption with The Modified Iron-Mesoporous Silica SBA-15 | Desita1, Mmaria Ulfa1, TeguhEndah Saraswati2 And Bakti Mulyani1 |
| JCC2017237 | Molecular Docking Simulation of Neuraminidase Influenza a Subtype H1N1 with Potential Inhibitor of Disulfide Cyclic Peptide (DNY, NNY, LRL) | Usman Sumo Friend Tambunan1, Riski Imaniastuti1, MochammadArfinFardiansyah Nasution1, Djati Kerami2 |
| JCC2017240 | Analysis of Hydrogen Gas Production from Seawater Electrolysis Using Variation of Voltage | Yoyon Wahyono1, Heri Sutanto1, Eko Hidayanto1, Ladaina Noura1, Eko Siswoyo2 |
| JCC2017244 | Aluminium - Cobalt-Pillared for Dye Filtration Membrane | Adi Darmawan1, Widiarsih1 |
| JCC2017247 | Fractionation of Glucomannan, New Hope for Corneal Lamellar Laceration Therapy, “A Preliminary Study” | A. Kartiwa1, M. Prayoga1, S. Heryati1, N. Atik2, D. Sariawati2, S. Bardi3, M. Fadhillah4, T. Subroto4 |
| JCC2017248 | Characterization of ZnO Nanoparticles from Waste Galvanized by Using Acetic Acid Extraction Followed by Precipitation | RismaDewi Dahlianti1, AprianRudina Sukma2, Iftitah3, Daisman P. Bayuaji1, Dody Prayitno1, Ersan Y. Muhlis1 |

| REG. CODE | Title | Author(s) |
|---|---|---|
| JCC2017298 | Carp Operculum Bone (CyprinusCarprio Sp.) Scaffold is A Potential Xenograft Implant Material: A Histological Study | A Kartiwa1, B Abbas2, P Pandansari2, N Atik3, RAA Syamsunarno4, SF Boesoirie1, MR Dahlan1, K Boesoirie1, A Prahasta1, M Nandini5, M Fadhillah6, A Switania1, T Subroto6 and R Panigoro4 |
| JCC2017300 | Photodegradation of Methyl Violet Using Graphite/PbTiO3 Composite | C. Purnawan1, S. Wahyuningsih2, V. Nawakusuma2 |
| JCC2017301 | Synthesis and Characterization of Bismuth Oxide using Sol Gel Method | Yayuk Astuti1, Darul Amri1, Krisna Dian Purnama1, Fauzan Musthafa1, Agus Muslim1, Arnelli1 |
| JCC2017302 | Ascorbic Acid Encapsulation in Silica Gel from Teos/Mtes Precursor by Sol-Gel Process | Sriyanti1, Sriatun1 |
| JCC2017303 | Method of ERASI (Electro Assisted Phytoremediation-Aeration) with Vetiveira Grass (Vetiveira Zizaniodes L) As Remediation of Heavy Metal Waste Fe and Cu | Iis Setianingrum1, EgaDwi Sintadani1, Vivin Viani1, Durrotul Uuliyah1, Muhammad FaiqFaridani2, Rudy Syah Putra3 |
| JCC2017304 | Identification of Flavonoid Compounds from the Active Fraction of the α-Glucosidase Inhibitor from Carrot Leaves Extract (Daucuscarota L.) | Khairul Anam1,FatikhaAulia Said1, Dewi Kusrini1 |
| JCC2017305 | A New Sorbent of Silica Magnetite: The Influence of Variation of Sodium Silicate Concentration on The Character of The Silica Magnetite | C Azmiyawati1, S Farnola1 and A Darmawan1 |
| JCC2017306 | Effect of Potentials and Electric Charges Copper and Indium Depositions to The Photocurrent Responses of CuInS2 Thin Film Fabricated By Stack Electrodeposition Followed by Sulfurization | Gunawan1, Abdul Haris1, Hendri Widiyandari2, Wilman Septina3, Shigeru Ikeda4 |
| JCC2017307 | Synthesis of 4-hydroxy-3-methylchalcone from Reimer-Tiemann Reaction Product and Its Antibacterial Activity Test | Mutiara Hapsari1, Tri Windarti1, Purbowatiningrum1, Ngadiwiyana1, Ismiyarto1 |
| JCC2017308 | Antiglycation and α-Glucosidase Inhibitory Properties of Alpiniapurpurata K Schum Fermented by Aspergillusniger | Agustina L. N. Aminin1, Ratnasari1, Meiny Suzery1, Bambang Cahyono1 |
| JCC2017309 | Synthesis and Characterization of NaCo(1-x)MnxO2 Solid Electrolyte Using Sol-Gel Method: The Effect of Milling Speed Variations | Linda Suyati1, OksitaAsri Widyayanti1, Muhammad Qushoyyi1, Rahmad Nuryanto1 |
| JCC2017310 | The Impact of Template Types on Polieugenol to The Adsorption Selectivity of Ionic Imprinted Polymer (Iip) Ion Metal Fe | Muhammad Cholid Djunaidi1, Abdul Haris1, Pardoyo1, Rosdiana K1 |
| JCC2017311 | Antidiabetic Activity from Cinnamaldydhe Encapsulated by Nanochitosan | Purbowatingrum1,Ngadiwiyana1, Enny Fachriyah, Ismiyarto, Bonita Ariestiani, Khikmah |

JCC2017167

# Golden Wattle (Acacia pycnantha) Flower: Is it Only Floral Emblem of Australia?

**Rudi Hendra**[1,2], **Paul Keller**[2]
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*Acacia pycnantha*, commonly known as the golden wattle, belongs to the Fabaceae family. Typically, it grows from 3 to 8 meters in height, and is native to New South Wales, Victoria, and South Australia.[1]Despite their bright colourful flowers, and that it is regarded as Australia's national flower, there are no reports on the structures present within the flower. Therefore, we present the phytochemical constituents in the flower, as well as correlations to their biological activities. The crude methanol were subjected to liquid-liquid extraction to provide hexane, ethyl acetate, and residual fractions. RP-HPLC profiles of both the ethyl acetate and residual fractions produced similar profiles. Thus, the ethyl acetate fraction was selected, and subjected to HPLC separation. Utilising the optimized preparative HPLC method, eight known compounds were isolated, and identified as (2*S*)-isohemiphloin (**1**),(2*S*)-naringenin-5-*O*-glucoside (**2**), kaempferol 3-rutinoside (**3**), quercetin 3-glucoside (**4**), myricetin 3-rhamnodise (**5**), kaempferol-3-rhamnoside (**6**), isosalipurposide (**7**), naringenin (**8**) by comparison of their spectral data with those reported in the literature. Furthermore, the extract and all isolated compounds were assessed for antibacterial activities against several human pathogenic bacteria by Hit-confirmation method with various results.

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# JCC2017179
# The Effect of Mangoosteen Extract (Gracinia Mangostana L.) on Synthesis of Ag3PO4 Photocatalyst

**Mohammad Afif[1], Alfa Marcorius[1], Khusnul Afifah[1], Siti Nurfiah[1], Khanifudin Khanifudin[2], Febiyanto Febiyanto[2], Uyi Sulaeman[1*]**
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Today, silver orthophosphate has been developed as phocatalyst for dye removal under visible light irradiation due to owing small-band gap energy of ~2.42 eV (1), strong photooxidative (2,3) and high quantum yield (3). The morphology and composites design have been applied to improve this photocatalyst. Morphology of saddle-like tetrahedron (4), coral-like microspheres (5), branched $Ag_3PO_4$ crystal with porous structure (6) and truncated tetragonal bipyramids (7) had improved the photocatalytic activity.

The big challenge of $Ag_3PO_4$ development is improvement the surface area and stability of photoreaction. The photocatalytic activity of $Ag_3PO_4$ is strongly affected by the size and surface area (8). Previous work showed that the synthesis of $Ag_3PO_4$ using PEG and PVP increased the specific surface area and enhanced the photocatalytic activity (9). Most of the preparation of $Ag_3PO_4$ catalyst using co-precipitation method resulted in low surface area. The poor performance of $Ag_3PO_4$ is attributed to the large particle size, which results in a low surface area, and thus low photocatalytic activity. Therefore, the development of the $Ag_3PO_4$ synthesis to design the small particle size is very important.

Herein, the $Ag_3PO_4$ prepared under mangoosteen (*Gracinia mangostana* L.) extract addition to the starting solution of $AgNO_3$ and $Na_2HPO_4.12H_2O$ could significantly decrease the particle size and increase the crystalline of $Ag_3PO_4$. This result enhances the photocatalytic activity. The mangoosteen extract solution of 0%, 1% and 1.5% were applied to producing the $Ag_3PO_4$ using the starting material of $AgNO_3$ and $Na_2HPO_4.12H_2O$. Samples were characterized using x-ray diffraction and scanning electron microscopy. Photocatalytic activities were evaluated using Rhodamine B photooxidation under blue light irradiation. The mangoosteen extract addition greatly decreases the particle size and increases the crystallinity of $Ag_3PO_4$ which significantly enhances the photocatalytic activity.

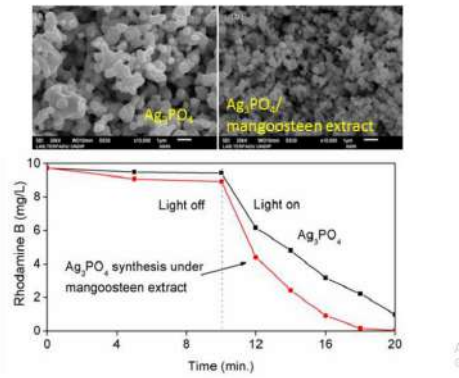


Fig. 1Morphology and Catalytic Activity

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JCC2017212

# Supramolecular Assembly of Group 11 Phosphorescent Metal Complexes for Chemosensors of Alcohol Derivatives

**Hendrik O. Lintang**[1,2,3], **Nur Fatiha Ghazalli**[4,5], **Leny Yuliati**[1,2,3]
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Transition metal complexes with phosphorescent properties have been utilized as chemical sensors (chemosensors) with high sensing capability for sensing different kinds of volatile organic compounds (VOCs). However, there is no study on molecular design of metal complexes toward high sensing capability. Therefore, by using 4-(3,5-dimethoxybenzyl)-3,5-dimethyl pyrazole ligand[1)] (**1e**) and group 11 metal ions (Cu(I), Ag(I), Au(I)), we report the systematic study on vapochromic sensing of VOCs such as alcohol derivatives using phosphorescent trinuclear pyrazolate complexes with supramolecular assembly of a weak intermolecular metal-metal interactions. Previously, the resulting trinuclear copper(I) 4-(3,5-dimethoxybenzyl)-3,5-dimethyl pyrazolate complex **2e**(**Cu**) revealed positive response to ethanol vapors by blue-shifting its emission band from 616 to 555 nm and emitting bright orange to green where the original intensity can be easily recovered and then reused without external stimuli.[2)] Moreover, **2e**(**Cu**) still showed the best performance for chemosensor of ethanol vapors compared to the same complexes synthesized from different side-chains at the pyrazole rings such as non-side chain, 3,5-dimethyl, 3,5-bis(trifluoromethyl), and 3,5-diphenyl pyrazole ligands.[3)] In this lecture, we particularly discuss the sensing capability of group 11 metal ions with the same ligand **1e**. Upon excitation at 284, the resulting complexes showed emission bands with a peak centered at 616, 473 and 612 nm for **2e**(**Cu**), **2e**(**Ag**) and **2e**(**Au**), respectively. Comparing to **2e**(**Cu**) with shorter metal-metal distance for sensing ethanol vapors in 5 mins, **2e**(**Au**) gave shifting from its emission band centered at 612 to 587 nm with $\Delta\lambda$ of 25 nm and color changes from red-orange to light green-orange. This blue-shifting was 41% compared to **2e**(**Cu**) with the same exposure time while the reusability testing required the presence of external stimuli. On the other hands, **2e**(**Ag**) with longer metal-metal distance showed quenching in its original emission intensity at 473 nm in 40% with color changes from dark green to less emissive. These results demonstrate that shifting phenomenon in **2e**(**Cu**) with the shorter metal-metal distance compared to **2e**(**Au**) from the same ligand is due to a weak intermolecular hydrogen bonding interaction of O atom at the methoxy of the benzyl ring with the OH of the vapors at the outside of the molecules. Such sensing phenomenon cannot be achieved for the detection of propanol, butanol, pentanol and hexanol vapors with decreasing in the performance to 37%, 28%, 23% and 18%, respectively, indicating suitable molecular design of ligand and metal ion in pyrazolate complex as chemosensor **2e**(**Cu**) for sensing ethanol vapors.

**References**

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JCC2017306

# Effect of Potentials and Electric Charges Copper and Indium Depositions to The Photocurrent Responses of CuInS2 Thin Film Fabricated By Stack Electrodeposition Followed by Sulfurization

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Effect of potentials and electric charges copper and indium depositions to the photocurrent responses of $CuInS_2$ thin film fabricated by electrodeposition followed by sulfurizationwere investigated. The characterization and elemental compositions of as-deposited Cu/In and $CuInS_2$ thin films used X-RD and EDAX. Photocurrent responses of the obtained $CuInS_2$ thin films were analyzed by linear sweep voltammograms (*LSV*s) in europium solution under chopped irradiation. Photocurrent responses showed that fabricated $CuInS_2$ thin films had *p*-type photoresponses. Improving potentials and electric charges reduced the photocurrent responses of the semiconductor films, alhough from XRD and EDAX data had no significant different.

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