

**LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH : JURNAL ILMIAH Jurnal Internasional Terindeks Pada Database Internasional
Bereputasi**

Judul Publikasi Ilmiah (Artikel) : **Computational Approach to Evaluate Eugenol Affinity and Derivatives Empirical Against Cu(II)**

Jumlah Penulis : 3 (tiga) orang

Status Penulis : Penulis Utama

Identitas Jurnal Ilmiah

a. Nama Jurnal Ilmiah : Molekul

b. Nomor ISBN /ISSN : ISSN : 1901-9761; e-ISSN : 2503-0310

c. Volume, Nomor, Bulan, Tahun : Volume 14 (2) November 2019

d. Penerbit : Jurusan Kimia FMIPA Unsud

e. DOI artikel : <https://doi.org/10.20884/1.jm.2019.14.1.467>

f. Alamat web jurnal : <https://ojs.jmolekul.com/ojs/index.php/jm>

g. Terindeks : di Mendeley, DOAJ, Scopus, Google, Crossref, IPI, Garuda, SINTA S1

h. Jumlah Halaman : 8 (148-155)

Kategori Publikasi Jurnal Ilmiah : **Jurnal internasional terindeks pada database internasional bereputasi**

Hasil Penilaian Peer Review

Komponen Yang Dinilai	Nilai Maksimal Jurnal Ilmiah			Nilai Akhir yang diperoleh
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	30			
a. Kelengkapan unsur isi jurnal (10%)	3			3
b. Ruang lingkup dan kedalaman pembahasan (30%)	9			9
c. Kecukupan dan kemutakhiran data/ informasi dan metodologi (30%)	9			8
d. Kelengkapan unsur dan kualitas penerbit (30%)	9			9
Total = (100 %)	30			29
Nilai Pengusul =	60%x29			17,4

Catatan Penilaian artikel oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi jurnal:**
Artikel sangat lengkap, dimana grafik dan tabel disitasi dan dibahas. Topik dan materi sesuai dengan jurnal yang bersangkutan. Tata penulisan tersaji dengan baik.
- Ruang lingkup dan kedalaman pembahasan:**
Artikel ini membahas tentang membandingkan antara studi komputasi dengan empiris. Metode disajikan secara terstruktur. Data-data ditampilkan dengan detail dan lengkap. Pembahasan dan interpretasi data dilakukan secara mendalam, serta cukup komprehensif dengan mensitasi referensi yang relevan.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:**
Referensi yang dicitasi dalam artikel ini ada 15 yang baru 7, Nilai novelty/kebaruan artikel termasuk agak kurang.
- Kelengkapan unsur dan kualitas terbitan:** Penerbit adalah Jurusan Kimia FMIPA Unsud, turnitin hanya 16%. Terindeks di Mendeley, DOAJ, , Google, Crossref, IPI, Garuda, SINTA S1. Kualitas penerbit sangat baik pada tingkat nasional.

Semarang, - 11 - 2019



Prof. Dr. Muhammad Djaeni, ST, MEng.
NIP. 197102071995121001
Unit kerja : Universitas Diponegoro
Jabatan Fungsional : Guru Besar
Bidang ilmu: Teknik Kimia

Nilai maksimum 25 jadi Nilai peer 1 (Prof Djaeni)

Menjadi $25/30 \times 17,4 = 14,5$

Nilai peer rata-rata = 14,36

Nilai PAK Universitas = 14,36

Ttd. Penilai PAK Universitas

Prof. Dr. Hadiyanto, ST, MSc

LEMBAR
HASIL PENILAIAN SEJAWAT SEBIDANG ATAU PEER REVIEW
KARYA ILMIAH : JURNAL ILMIAH (jurnal Nasional Terakreditasi)

Judul Publikasi Ilmiah (Artikel)	:	Computational Approach to Evaluate Eugenol Aff and Derivatives Empirical Against Cu(II)
Penulis Jurnal Ilmiah	:	Muhammad Cholid Djunaidi, Tantri Nevi Astuti, a Parsaoran Siahaan. (penulis 1)
Identitas Jurnal Ilmiah	a. Nama Jurnal Ilmiah:	Molekul
	b. Nomor ISBN /ISSN	ISSN : 1901-9761; e-ISSN : 2503-0310
	c. Volume, Nomor, Bulan, Tahun	Volume 14 (2) November 2019
	d. Penerbit	Penerbit :Jurusan Kimia FMIPA Unsud
	e. DOI artikel (jika ada)	https://doi.org.10.20884/1.jm.2019.14.1.467
	f. Alamat web jurnal	https://ojs.jmolekul.com/ojs/index.php/jm
	g. Terindeks di Mendeley, DOAJ, Scopus, Google, Crossref, IPI, garuda, SINTA S1	
	e. Jumlah Halaman	8 (148-155)

Kategori Publikasi Jurnal Ilmiah : Jurnal Ilmiah Nasional Terakreditasi
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Hasil Penilaian Peer Review

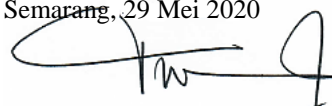
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a. Kelengkapan unsur isi jurnal (10%)		25		2,2
b. Ruang lingkup dan kedalaman pembahasan (30%)		7,5		7,1
c. Kecukupan dan kemutakhiran data/ informasi dan metodologi (30%)		7,5		7,1
d. Kelengkapan unsur dan kualitas penerbit (30%)		7,5		7,3
Total = (100 %)		25		23,7
Nilai Pengusul =				

Catatan Penilaian artikel oleh Reviewer :

- Kesesuaian dan kelengkapan unsur isi jurnal:**
 Jurnal telah ditulis lengkap dan sesuai dengan template, terdiri dari pendahuluan, metode, hasil dan pembahasan, kesimpulan serta referensi. Artikel berisi tentang pendekatan komputasi terhadap eugenol dan senyawa turunannya.
- Ruang lingkup dan kedalaman pembahasan:**
 Ruang lingkup adalah komputasi senyawa organik, pembahasan telah melakukan sitasi walaupun banyak dalam bentuk diskripsi.
- Kecukupan dan kemutakhiran data/informasi dan metodologi:**
 Data sangat memadai dan disajikan dengan baik referensi terkini sebanyak 33,33% dari referensi yang disajikan (ketika jurnal ini terbit)
- Kelengkapan unsur dan kualitas terbitan:**
 Kualitas penerbit yaitu jurusan kimia FMIPA Unsoed termasuk baik dan sudah terindeks, kualitas jurnal yang diterbitkan baik

Jabatan Fungsional: Guru Besar
 Bidang ilmu/Unit kerja :Teknik Kimia/ Universitas
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Semarang, 29 Mei 2020

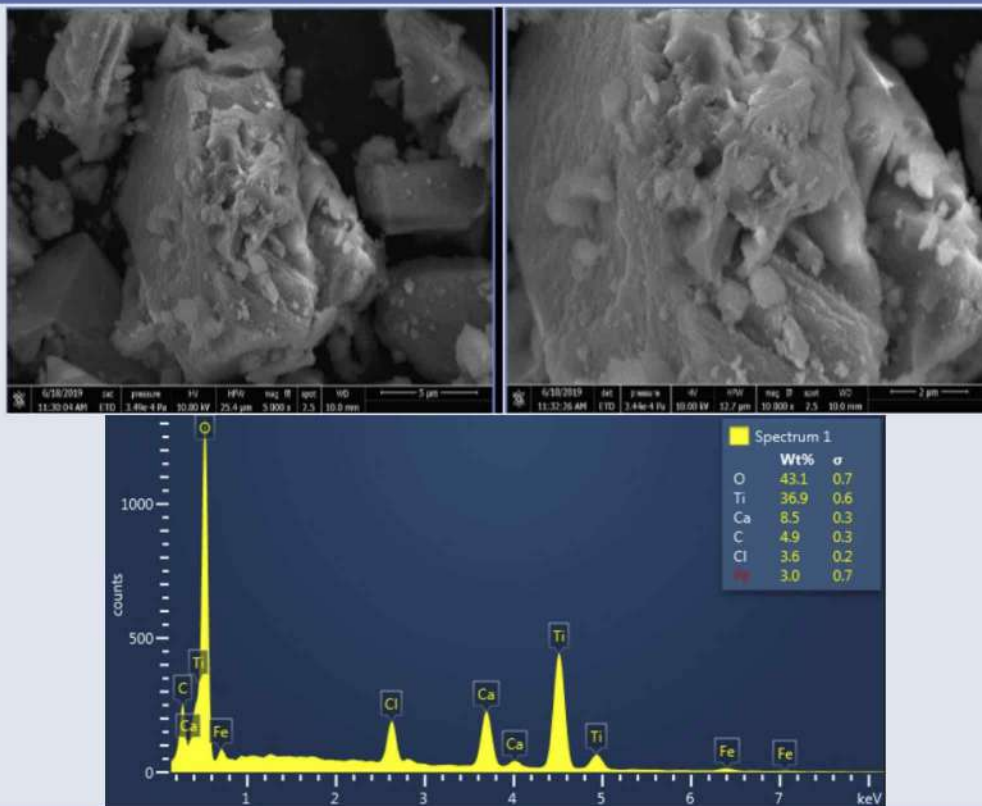


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 NIP. 19720906 199803 1001

Jurnal Ilmiah Kimia

MOLEKUL

Vol. 14, No. 2, November 2019



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Jurusan Kimia
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Jenderal Soedirman
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Molekul

Vol. 14

No. 2

pp. 78 - 148

Nov
2019P-ISSN
1907-9761E-ISSN
2503-0310



MOLEKUL

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Molekul

**Jurnal Ilmiah Kimia
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Scope](#)

[Publication
Ethics](#)

[Peer
Review
Process](#)

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[HOME](#) [ABOUT](#) [LOGIN](#) [REGISTER](#) [SEARCH](#) [CURRENT](#)

[ARCHIVES](#)

Home > Archives > **Vol 14, No 2 (2019)**

Vol 14, No 2 (2019)

Table of Contents

Articles

[Quantitative Structure-Property Relationship Analysis Against Critical Micelle Concentration of Sulfonate-Based Surfactant Based on Semiempirical Zindo/1 Calculation](#)

PDF
78-83

Ponco Iswanto, Eva Vaulina Yulistia Delsy, Ely Setiawan, Fiandy Aminullah Putra
| DOI : [10.20884/1.jm.2019.14.2.467](https://doi.org/10.20884/1.jm.2019.14.2.467) | This article has been viewed: **408 times** |

[Optimization of Total Flavonoids Extraction and A-Glucosidase Inhibitory Activity from Plectranthus amboinicus \(Lour.\) Spreng. Leaves using the Simplex-Centroid Design](#)

PDF
84-91

Kunto Wibisono, Syarifah Iis Aisyah, Sri Suhesti, Waras Nurcholis
| DOI : [10.20884/1.jm.2019.14.2.497](https://doi.org/10.20884/1.jm.2019.14.2.497) | This article has been viewed: **498 times** |

[The bioactive contents and antioxidant activity of honey bee nest extract of Apis dorsata Binghami from the North Sulawesi](#)

PDF
92-102

Mokosuli Yermia Samuel, Eva Sherly Nonke Kaunang, Jacklin Stella Manopo
| DOI : [10.20884/1.jm.2019.14.2.502](https://doi.org/10.20884/1.jm.2019.14.2.502) | This article has been viewed: **461 times** |

[β-Sitosterol and Betulonic Acid from n-Hexane Extract the Stem Bark of Tetracera indica](#)

PDF
103-109

Muharni Muharni, elfita elfita, Julinar Julunar, Heni Yohandini, muthia oktaviani
| DOI : [10.20884/1.jm.2019.14.2.507](https://doi.org/10.20884/1.jm.2019.14.2.507) | This article has been viewed: **383 times** |

[Effectiveness of Leaves Extract Fractions of Archidendron jiringa \(Jack\) I.C Nielsen Against Microbes](#)

PDF
110-116

Oom Komala, Sri Wardatun, Lia Puspita Sari
| DOI : [10.20884/1.jm.2019.14.2.538](https://doi.org/10.20884/1.jm.2019.14.2.538) | This article has been viewed: **605 times** |

[No Acute Toxicity Tests of Purwoceng \(Pimpinella pruatjan Molck.\) Ethanolic Extract on Male Albino Rat by Determined Hepatorenal Function Test and Histopathology.](#)

PDF
117-125

Fitranto Arjadi, Dhadhang Wahyu Kurniawan, Yudhi Wibowo, Wahyu Siswandari, Lantip Rujito

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[Plagiarism Policy](#)

Abstract Indexed in:

Scopus[®]



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| DOI : [10.20884/1.jm.2019.14.2.542](https://doi.org/10.20884/1.jm.2019.14.2.542) | This article has been viewed: **311 times** |

[Caryophyllene-Type Sesquiterpenoids from the Stembark of *Aglalia harmsiana* and Their Cytotoxic Activity Against MCF-7 Breast Cancer Cells](#)

Hersa Milawati, Desi Harneti, Rani Maharani, Nurlelasari Nurlelasari, Ace Tatang Hidayat, Mohamad Nurul Azmi, Yoshihito Shiono, Unang Supratman

| DOI : [10.20884/1.jm.2019.14.2.543](https://doi.org/10.20884/1.jm.2019.14.2.543) | This article has been viewed: **313 times** |

[Xylose and Arabinose Fermentation to Produce Ethanol by Isolated Yeasts from Durian \(*Durio zibethinus L.*\) Fruit](#)

Hermansyah Hermansyah, Fachrijal Fachrijal, Miksusanti Miksusanti, Fatma Fatma, Getari Kasmiarti, Almunadi T Panagan

| DOI : [10.20884/1.jm.2019.14.2.562](https://doi.org/10.20884/1.jm.2019.14.2.562) | This article has been viewed: **183 times** |

[Synthesis and Characterization of TiO₂-CaO and TiO₂-CaO-Fe₂O₃ Photocatalyst for Removal of Catechol](#)

Candra Yulius Tahya, Wahyu Irawati, Karnelasatri Karnelasatri, Friska Juliana Purba

| DOI : [10.20884/1.jm.2019.14.2.570](https://doi.org/10.20884/1.jm.2019.14.2.570) | This article has been viewed: **446 times** |

[Computational Approach to Evaluate Eugenol Affinity and Derivatives Empirical Against Cu\(II\)](#)

Muhammad Cholid Djunaedi, Tantri Nevi Astuti, Parsaoran Siahaan

| DOI : [10.20884/1.jm.2019.14.2.499](https://doi.org/10.20884/1.jm.2019.14.2.499) | This article has been viewed: **155 times** |

[Toxicity test of desorbed chromium from polluted soil around tannery industry in Yogyakarta-Indonesia by using *Brassica juncea* and *Helianthus annuus L.*](#)

Suherman Suherman, Wina Akmarina, Wulandari Sutiawan, Nurul Hidayat Aprilita, Mudasir Mudasir, Kinichi Morita

| DOI : [10.20884/1.jm.2019.14.2.557](https://doi.org/10.20884/1.jm.2019.14.2.557) | This article has been viewed: **222 times** |



PDF
126-132



[Detail Statistic](#)

PDF
133-139

USER

Username

Password

Remember me

PDF
140-148

PDF
149-156

PDF
157-163

Editorial

[Frontmatter \(Front Cover, Editorial Team, Preface and Table of Contents\)](#)

PDF

[Backmatter \(Instruction for author and back cover\)](#)

PDF



Molekul

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KEMENTERIAN RISET DAN TEKNOLOGI/BADAN RISET
DAN INOVASI NASIONAL
DEPUTI BIDANG PENGUATAN RISET DAN PENGEMBANGAN
Gedung B.J.Habibie Lantai 19 – 20, Jalan M.H. Thamrin No. 8, Jakarta 10340
Telepon 021-3162222 Ext. 9702, 9782, 9707; Faksimile 021-3101728

Nomor : B/804/E5/E5.2.1/2019
Lampiran : 1 (satu) Berkas
Perihal : **Pemberitahuan Hasil Akreditasi Jurnal Ilmiah
Periode I Tahun 2020**

Jakarta, 3 April 2020

Kepada Yth.

1. Pimpinan Perguruan Tinggi
2. Koordinator LL Dikti I s.d. XIV
3. Ketua Himpunan Profesi
4. Pengelola Jurnal Ilmiah
di seluruh Indonesia

Dengan hormat,

Sehubungan dengan hasil Akreditasi Jurnal Ilmiah Periode I Tahun 2020 dan telah diterbitkannya Surat Keputusan Menteri Riset dan Teknologi/Badan Riset dan Inovasi Nasional Nomor 85/M/KPT/2020, tanggal 01 April 2020, dengan hormat bersama ini kami sampaikan hasil akreditasi sebagaimana terlampir. Adapun ketentuan penerbitan sertifikat akreditasi sebagai berikut:

1. Bagi usulan akreditasi baru maka sertifikat akreditasi akan diterbitkan dan diberikan kepada pengelola jurnal.
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3. Bagi usulan akreditasi ulang yang hasil akreditasi peringkatnya tetap dan telah memiliki sertifikat yang masih berlaku masa akreditasi, maka sertifikat baru tidak akan diterbitkan, dan sertifikat sebelumnya dapat digunakan sampai berakhir masa berlaku.
4. Bagi pengelola yang sudah terakreditasi dan namanya tercantum dalam SK sebelumnya serta belum memiliki sertifikat dapat meminta sertifikat terdahulu.
5. Penerbitan sertifikat dilakukan secara bertahap paling cepat 2 minggu setelah pengumuman ini dan dilakukan pemutakhiran data di laman : <http://sinta2.ristekbrin.go.id/journals>, penyerahan sertifikat dilakukan secara bertahap dapat diunduh langsung melalui akun pengusul di laman: <http://arjuna.ristekbrin.go.id/> mulai tanggal 6 Juni 2020.
6. Bagi usulan yang ditolak administrasi dan usulan baru bisa mengajukan kembali melalui <http://arjuna.ristekbrin.go.id/>.

Atas perhatian dan kerja sama yang baik, kami ucapkan terima kasih.

Direktur Pengelolaan Kekayaan Intelektual

ttd

Heri Hermansyah
NIP. 197601181999031002

Tembusan :
Plt. Deputi Bidang Penguatan Riset dan Pengembangan



SALINAN

**MENTERI RISET DAN TEKNOLOGI/
KEPALA BADAN RISET DAN INOVASI NASIONAL
REPUBLIK INDONESIA**

KEPUTUSAN MENTERI RISET DAN TEKNOLOGI/
KEPALA BADAN RISET DAN INOVASI NASIONAL
REPUBLIK INDONESIA

NOMOR 85/M/KPT/2020

TENTANG

PERINGKAT AKREDITASI JURNAL ILMIAH PERIODE I
TAHUN 2020

MENTERI RISET DAN TEKNOLOGI/
KEPALA BADAN RISET DAN INOVASI NASIONAL
REPUBLIK INDONESIA,

- Menimbang : a. bahwa dalam rangka pembinaan dalam penyelenggaraan ilmu pengetahuan dan teknologi serta untuk meningkatkan relevansi, kuantitas, dan kualitas publikasi ilmiah ilmuwan Indonesia untuk mendukung daya saing bangsa diperlukan peringkat akreditasi jurnal ilmiah;
- b. bahwa berdasarkan hasil akreditasi jurnal ilmiah yang ditetapkan oleh Tim Akreditasi Jurnal Ilmiah Kementerian Riset dan Teknologi/Badan Riset dan Inovasi Nasional pada tanggal 26 Maret 2020, telah diperoleh Peringkat Akreditasi Jurnal Ilmiah Periode I Tahun 2020;
- c. bahwa berdasarkan pertimbangan sebagaimana dimaksud dalam huruf a dan huruf b, perlu menetapkan Keputusan Menteri Riset dan Teknologi/Kepala Badan Riset dan Inovasi Nasional tentang Peringkat Akreditasi Jurnal Ilmiah Periode I Tahun 2020;
- Mengingat : 1. Undang-Undang Nomor 12 Tahun 2012 tentang Pendidikan Tinggi (Lembaran Negara Republik Indonesia Tahun 2012 Nomor 158, tambahan Lembaran Negara Republik Indonesia Nomor 5336);

2. Undang-Undang ...

2. Undang-Undang Nomor 11 Tahun 2019 tentang Sistem Nasional Ilmu Pengetahuan dan Teknologi (Lembaran Negara Republik Indonesia Tahun 2019 Nomor 148, Tambahan Lembaran Negara Republik Indonesia, Tambahan Lembaran Negara Republik Indonesia Nomor 6374);
3. Peraturan Pemerintah Nomor 4 Tahun 2014 tentang Penyelenggaraan Pendidikan dan Pengelolaan Perguruan Tinggi (Lembaran Negara Republik Indonesia Tahun 2014 Nomor 16, Tambahan Lembaran Negara Republik Indonesia Nomor 5500);
4. Peraturan Presiden Nomor 50 Tahun 2020 tentang Kementerian Riset dan Teknologi (Lembaran Negara Republik Indonesia Tahun 2020 Nomor 89);
5. Keputusan Presiden Nomor 113/P Tahun 2019 tentang Pembentukan Kementerian Negara dan Pengangkatan Menteri Negara Kabinet Indonesia Maju Periode Tahun 2019-2024;

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Menetapkan : KEPUTUSAN MENTERI RISET DAN TEKNOLOGI/KEPALA BADAN RISET DAN INOVASI NASIONAL TENTANG PERINGKAT AKREDITASI JURNAL ILMIAH PERIODE I TAHUN 2020.

KESATU : Menetapkan Peringkat Akreditasi Jurnal Ilmiah Periode I Tahun 2020 sebagaimana tercantum dalam Lampiran yang merupakan bagian yang tidak terpisahkan dari Keputusan Menteri/Kepala Badan ini.

KEDUA : Akreditasi Jurnal Ilmiah sebagaimana dimaksud dalam Diktum KESATU berlaku selama 5 (lima) tahun mulai dari nomor dan tahun sebagaimana tercantum dalam Lampiran yang merupakan bagian yang tidak terpisahkan dari Keputusan Menteri/Kepala Badan ini.

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Ditetapkan di Jakarta
pada tanggal 1 April 2020


MENTERI RISET DAN TEKNOLOGI/
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NASIONAL REPUBLIK INDONESIA,

ttd.

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BADAN RISET DAN INOVASI NASIONAL
Sekretariat Kementerian/Sekretariat Utama
Kepala Biro Hukum dan Organisasi,




Ardhen Nissa Widhawati Siswojo

SALINAN

LAMPIRAN

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KEPALA BADAN RISET DAN INOVASI NASIONAL
REPUBLIK INDONESIA
NOMOR 85/M/KPT/2020
TENTANG
PERINGKAT AKREDITASI JURNAL ILMIAH
PERIODE I TAHUN 2020

PERINGKAT AKREDITASI JURNAL ILMIAH PERIODE 1 TAHUN 2020

Peringkat	No.	Nama Jurnal	E-ISSN	Penerbit	Keterangan
1	1	<i>Bulletin of Chemical Reaction Engineering & Catalysis</i>	19782993	<i>Departement of Chemical Engineering, Diponegoro University</i>	Reakreditasi Tetap di Peringkat 1 mulai Volume 15 Nomor 1 Tahun 2020
	2	<i>Indonesian Aquaculture Journal</i>	25026577	<i>The Center for Fisheries Research, Indonesian Ministry of Marine Affairs and Fisheries</i>	Reakreditasi Tetap di Peringkat 1 mulai Volume 14 Nomor 2 Tahun 2019
	3	<i>Indonesian Journal of Chemistry</i>	24601578	<i>Chemistry Department, Faculty of Mathematics and Natural Sciences, Universitas Gadjah Mada</i>	Reakreditasi Tetap di Peringkat 1 mulai Volume 20 Nomor 1 Tahun 2020
	4	Jurnal Ilmu Ternak dan Veteriner	2252696X	<i>Indonesian Center for Animal Research and Development</i>	Reakreditasi Tetap di Peringkat 1 mulai Volume 24 Nomor 4 Tahun 2020
	5	<i>Kesmas: National Public Health Journal</i>	24600601	Fakultas Kesehatan Masyarakat Universitas Indonesia	Reakreditasi Tetap di Peringkat 1 mulai Volume 14 Nomor 2 Tahun 2019

Peringkat	No.	Nama Jurnal	E-ISSN	Penerbit	Keterangan
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Computational Approach to Evaluate Eugenol Affinity and Derivatives Empirical Against Cu(II)

by Muhammad Cholid Djunaidi

Submission date: 03-Jun-2020 05:20PM (UTC+0700)

Submission ID: 1337017081

File name: C_23_molekul.pdf (399.6K)

Word count: 3571

Character count: 18914

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Received March 6, 2019; Accepted October 10, 2019; Available online November 30, 2019

ABSTRACT. A computational approach to assess the empirical results of eugenol affinity, eugenol acetate (EOA), and pyridine methyl eugenol acetate (PMEOA) against Cu²⁺ has been done. This research aims to determine the effects of the functional groups (–OH, –COOH, and –N) on eugenol and their derivatives on the selectivity of Cu²⁺ adsorption experimentally and to calculate the energy interaction between eugenol compounds and derivatives with Cu²⁺. The experimental approach was carried out by solvent extraction method, using 10 mL of Cu²⁺ 10 ppm solution along with 0.3089 mmol of eugenol, EOA and PMEOA. The remaining concentration of Cu²⁺ metal after extraction in the water phase was measured using an Atomic Absorption Spectrophotometer (AAS). Assessments of the Cu²⁺ metal interaction with eugenol, EOA and PMEOA compounds were carried out using the ab initio method with 6-31G** basis set to predict the interaction energy. The results showed that pyridine methyl eugenol acetate (PMEOA) can separate Cu²⁺ better than eugenol and EOA with extraction efficiency (% E) = 78.76%. The calculation results of Cu²⁺ metal interactions with eugenol, EOA, and PMEOA compounds found that PMEOA has the lowest energy of interaction compared to eugenol and EOA with Cu²⁺ metal.

Keywords: Eugenol, Eugenol Derivatives, AAS, Ab Initio, affinity, Cu²⁺, solvent extraction

INTRODUCTION

The industry is currently experiencing very rapid development. However, the result of the rapid development of the industry is the production of waste in the form of solid, liquid and gas wastes which result in environmental pollution. Liquid waste in the industry has a role in the release of heavy metals into the water flow. This creates a negative impact on living things in the environment. One of the heavy metals that can pollute the environment is Cu. Metal Cu above the permitted threshold will cause poisoning to living things, especially in humans, potentially causing death. Therefore, it is necessary to tackle pollution caused by Cu metal. Efforts to control and process heavy metal waste are developing, leading to the searches for new methods that are cheap, effective and efficient (Kundari & Slamet, 2012).

A method that can be used to process heavy metal waste is liquid-liquid extraction. Extraction is highly significant in selective metal separation techniques in industrial waste treatment processes (Khoutoul et al., 2016). Liquid-liquid extraction is the commended technique to recover metals (Hamzah et al., 2011). Moreover, the chosen extraction method has advantages in its use as it does not require expensive

and complicated equipment (Harimu, Matsjeh, Siswanta, & Santosa, 2009). The basic principle of liquid-liquid extraction involves contacting a solution with other solvents that are not immiscible with the original solvent with different density so that it will form two phases shortly after the solvents are combined (Mirwan & Wicakso, 2008)

The latest development of extraction separation method tends to increase selectivity to certain metals by finding new ligands as extractants through compound synthesis (Kakoi et al., 1998). One of the raw materials that can be used is eugenol. Eugenol is a natural component found in essential oils, including cloves. The content of eugenol in cloves ranges from 60-90% (Sneddon, 1997). Eugenol is an Indonesian natural ingredient that can be used for the separation of metal ions (Djunaidi, Jumina, Siswanta, & Ulbricht, 2015; Djunaidi, Siswanta, & Jumina, 2015). Eugenol is used as a starting material for the synthesis of a compound because there are three functional groups that are bound to it, namely the allyl, hydroxyl and methoxy groups that can potentially work as functional monomers for the selective adsorption process of Cu (Djunaidi, Wibawa, & Murti, 2018). With these three active groups, eugenol can function as a carrier

through a hydroxyl group where eugenol can be entered into a more selective functional group. To increase the selectivity of eugenol, modification was carried out to improve the selectivity of eugenol (Djunaidi, Khabibi, & Khrisna, 2010). In this study, modification was done by synthesizing eugenol derivatives in the form of eugenoxo acetic acid (EOA) and pyridine methyl eugenoxo acetate (PMEOA).

In addition to the synthesis of eugenol derivatives, this study also aims to study the interaction of Cu^{2+} with eugenol, EOA, and PMEOA molecules, calculate the interaction energy between eugenol compounds and eugenol derivatives with the most stable Cu^{2+} in silico. The experimental approach is carried out by solvent extraction methods. The concentration of Cu^{2+} metal remaining after extraction in the liquid phase was measured using Atomic Absorption Spectrophotometer (AAS). Evaluation of the interactions of Cu^{2+} metal with eugenol, EOA, and PMEOA compounds were carried out using the *ab initio* method with basis set 6-31G** to predict the interaction energy. Through the *ab initio* method in this study, computational prediction of the interactions can be found and compared to existing theories and experimental results.

EXPERIMENTAL SECTION

Materials

Eugenol pa (SIGMA Aldrich), technical grade Na_2SO_4 (Merck), HCl (Merck), NaHCO_3 (Merck), NaOH pa (Merck), ClCH_2COOH pa (Merck), Chloroform pa (Merck), Aqua Bidest, $\text{Cu}(\text{NO}_3)_2$ (Merck), 2-Pyridinemethanol pa (SIGMA Aldrich), Thionyl Chloride pa (Merck).

Instruments

Laboratory glassware, reflux equipment, analytical balance sheet (Mettler-200), magnetic stirrer, hotplate stirrer, spatula, pH meter, fine filtering paper, AAS (Perkin Elmer), FTIR (8201PC Shimadzu), a set of computers with Linux and Windows OS, Notepad ++ software, Chemcraft Software, and Nwchem 6.3 software.

Methodology

Eugenoxo Acetic Acid Synthesis

Five grams of eugenol were put into a 100 mL boiling flask and was added with 17.5 mL of 33% NaOH solution. The mixture was stirred for 30 minutes. Then 12.5 mL of 50% chloroacetic acid solution was added gradually using a dropping pipette while it continued to be stirred. The mixture was heated in a water bath at a temperature of 80-90 °C. Heating was carried out for 2 hours and the process proceeded to cooling and acidification using 6 M HCl to obtain pH=1. The next stage was extraction using 50 mL

diethyleter with 2 repetitions. The ether extracted was combined and extracted again using sodium bicarbonate 5% b/v as much as 30 mL with 3 repetition. The layer of water was then acidified with 6 M HCl to attain pH=1. Filtering, drying, and weighing were carried out. The results obtained were analyzed using FTIR.

Pyridine Methyl Eugenoxo Acetate Synthesis

A total of 3 g (0.0135 mol) of eugenoxo acetic acid (EOA) was put into a 100 mL boiling flask. The EOA was added with 1.6 mL (2.624 g, 0.022 mol) thionyl chloride dropwise. Then the mixture was refluxed for 150 minutes in a warm cooking oil bath (40 °C), and then cooled. Into the mixture 2 mL (2.262 g, 0.0207 mol) of pyridylcarbinol was added dropwise and refluxed again in warm cooking oil (40 °C) for 60 minutes. After it had cooled the result obtained was dissolved in chloroform and washed with water. The extraction result was dried with sodium sulfate anhydride, filtered and then evaporated to remove the remaining solvent. Furthermore, the results were analyzed using FTIR.

Liquid-liquid Extraction

A sample with a concentration of 0.000638 mol was dissolved in 10 mL of chloroform and extracted with 10 mL of 10 ppm Cu(II) ion for 3 hours. The mixture was separated and the Cu(II) concentration in the filtrate was analyzed using AAS twice.

Computational Method

Nwchem 6.3 program was used for all *ab initio* molecular orbital and self-consistent field calculations. The geometry of eugenol, EOA and PMEOA, and Cu^{2+} metal ions were optimized at the 6-31G** basis set. The energy of intermolecular interactions of molecules was also calculated by the SCF method with the same basis for the *ab initio* calculation.

RESULTS AND DISCUSSION

Eugenoxo Acetic Acid (EOA) Synthesis

The results of the analysis using an infrared spectromete are obtained according to Figure 1. The presence of absorption bands at 3400 and 3500 cm^{-1} indicate the presence of -OH groups in carboxylic acids. Absorption bands in the range 3100-3000 cm^{-1} are C-H sp bands, the range 1600-1475 cm^{-1} is vibrations of C=C from the aromatic ring and the range 800-900 cm^{-1} indicate that the aromatic is substituted. Uptake at 1635 cm^{-1} , 997 cm^{-1} , and 915 cm^{-1} are the absorption of vinyl groups (RHC = CH). Acid carboxyl groups are shown in absorption at 1728.22 cm^{-1} .

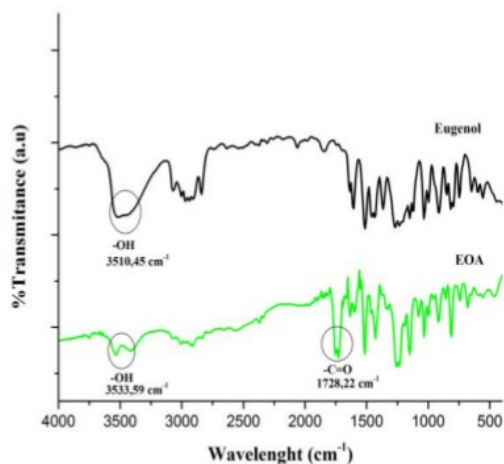
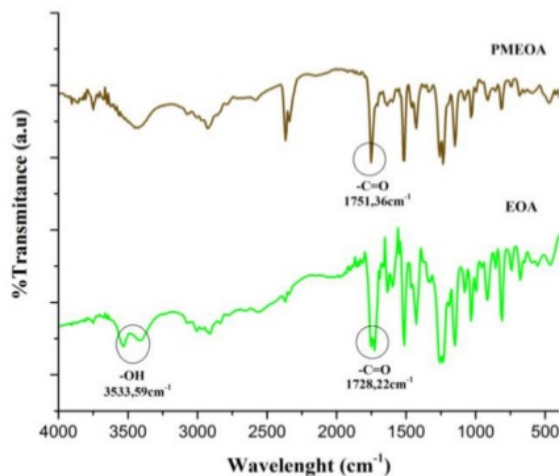


Figure 1. FTIR Spectra of Eugenol and EOA



13
Figure 2. FTIR Spectra of EOA and PMEOA

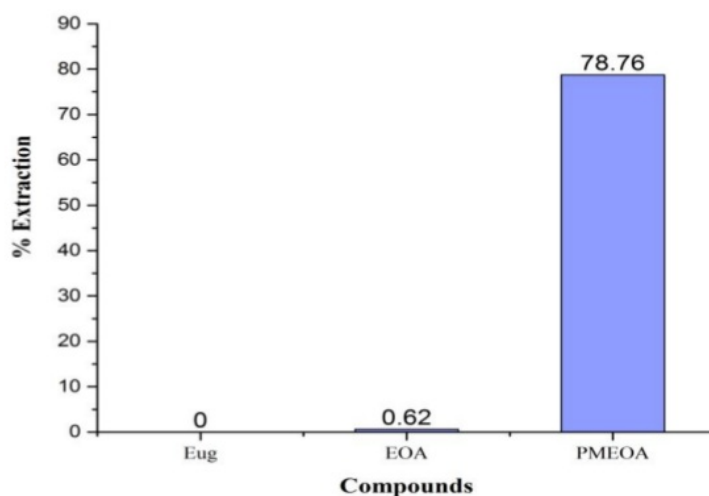


Figure 3. Results of Cu^{2+} metal % Extracted in Eugenol, EOA, and PMEOA

EOA was purified by extraction using diethyleter to remove polar impurities along with extraction using NaHCO_3 to remove nonpolar impurities. The synthesized EOA has a yield of 75.73%, in the form of a brownish white precipitate and has a melting point of 88-93 °C. The results of the EOA synthesis produced are in accordance with previous studies (Djunaidi et al., 2010).

Pyridine Methyl Eugenoxy Acetate (PMEOA) Synthesis

PMEOA was obtained from EOA based synthesis. The results of PMEOA synthesis can be seen from the results of the following FTIR analysis, Figure 2. The

formation of ester can be identified from the infrared spectra at wave number $1751,36 \text{ cm}^{-1}$ which is a spectrum of the carbonyl ester group. Another proof of the formation of esters is the loss of characteristic spectra of the $-\text{OH}$ group or hydrogen bonds which form a wide band at a wavenumber of about 3500 cm^{-1} (Djunaidi et al., 2018). The experiment obtained PMEOA with a yield of 75,73%.

Cu^{2+} Metal Extraction Results

From [21] experimental outcome obtained, %extracted results are shown in Figure 3. Based on Figure 3 above, it appears that the percentage of $\text{Cu}(\text{II})$

metal ions extracted was highest in PMEOA, followed by EOA and last, eugenol. This is in accordance with the HSAB (Hard Soft Acid Base) theory that says hard acid metals bind more strongly with hard bases, soft acids with soft bases, and borderline acids with

borderline bases. Cu(II) is a borderline acid metal ion so that it can bind to the N-active ligand which is a stronger borderline base than other metal ions (Ho, 1975).



Figure 4. (a) Optimized Geometry of Eugenol (b) Eugenoxo Acetate (EOA) (c) Pyridine Methyl Eugenoxo Acetate

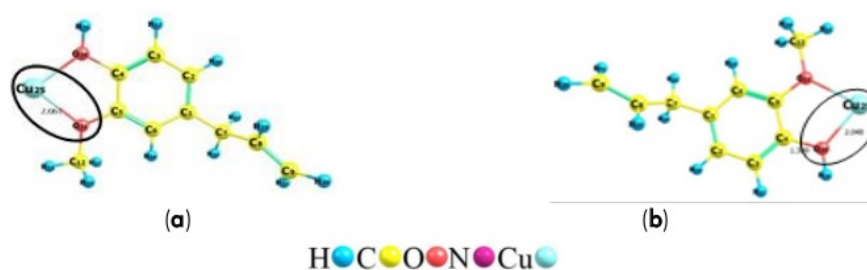


Figure 5. Optimized Geometry of interaction between Eugenol and Cu^{2+} (a) Eugenol O_{10} atom Cu^{2+} (b) Eugenol O_{11} atom Cu^{2+}

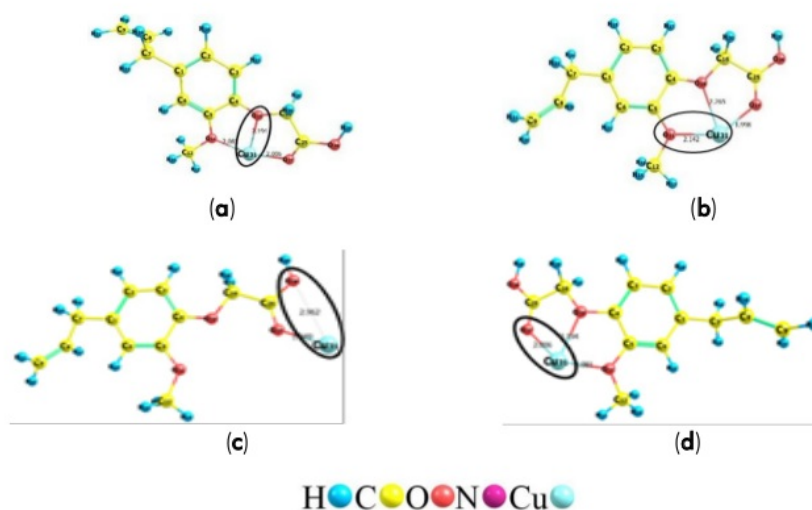


Figure 6. Geometry optimization of eugenoxo acetate (EOA) that has interacted with Cu^{2+} (a) EOA O_{10} atom Cu^{2+} (b) EOA O_{11} atom Cu^{2+} (c) EOA O_{26} atom Cu^{2+} (d) EOA O_{27} atom Cu^{2+}

Computational Study

In this study, Cu^{2+} was exposed and interacted with eugenol, EOA, and PMEOA molecules. The atoms that interacted with Cu^{2+} in eugenol were O_{10} and O_{11} , in EOA were O_{10} , O_{11} , O_{26} and O_{27} whereas in PMEOA were O_{10} , O_{11} , O_{26} , O_{27} , and N_{32} atoms. The results of geometry optimization show that there are interactions between Cu^{2+} with eugenol, EOA and PMEOA, **Figure 4.** and **Table 1,** which were indicated by changes in distance, angle, and dihedral in each molecule shown in **Table 2.**

The interactions were carried out at the positions of the eugenol O_{10} atom $\dots\text{Cu}^{2+}$ and eugenol O_{11} atom $\dots\text{Cu}^{2+}$ which produced interaction energies that are not much different, specifically $\text{O}_{10} \dots\text{Cu}^{2+}$ at -766.554 kJ/mol and $\text{O}_{11} \dots\text{Cu}^{2+}$ at -766.523 kJ/mol. Energy of the resulting interactions is not much different because $\dots\text{Cu}^{2+}$ interacts with O_{10} and O_{11} producing energies that are not much different. However, the stability generated from the O_{10} atomic interaction with Cu^{2+} tends to be greater because O_{11} has a larger steric effect thus $\dots\text{Cu}^{2+}$ interacts better with O_{10} (**Figure 5.b**) (Warren, 1981).

The interactions that occur in the EOA molecule take place in the positions of $\text{O}^{10} \dots\text{Cu}^{2+}$, $\text{O}_{11} \dots\text{Cu}^{2+}$, $\text{O}_{26} \dots\text{Cu}^{2+}$, $\text{O}_{27} \dots\text{Cu}^{2+}$ which produced energy of interactions of -879.662 kJ/mol, -877.986 kJ/mol, -859.391 kJ/mol, and -879.661 kJ/mol, respectively. Geometry optimizations of interaction structures obtained the most stable energy in the interaction of O_{10} EOA atom with $\dots\text{Cu}^{2+}$ as it has the greatest interaction energy compared to the others (Zhai et al., 2018). This is because in that position Cu^{2+} interacts a lot more creating stronger interaction (**Figure 6.a**).

Molecular interaction positions between PMEOA and Cu^{2+} namely $\text{O}_{10} \dots\text{Cu}^{2+}$, $\text{O}_{11} \dots\text{Cu}^{2+}$, $\text{O}_{26} \dots\text{Cu}^{2+}$, and $\text{O}_{27} \dots\text{Cu}^{2+}$ produced interaction energies of -1042.046 kJ/mol, -1042.044 kJ/mol, -990.714 kJ/mol, -912.450 kJ/mol and -995.279 kJ/mol, respectively. The greatest interaction energy sign on the molecular geometry optimization results states stable molecular structure (Yopianto, et al., 2011). Accordingly, the most powerful interaction of the PMEOA molecule is at the position $\text{O}_{14} \dots\text{Cu}^{2+}$ as it produces the greatest interaction energy (**Figure 7.a**).

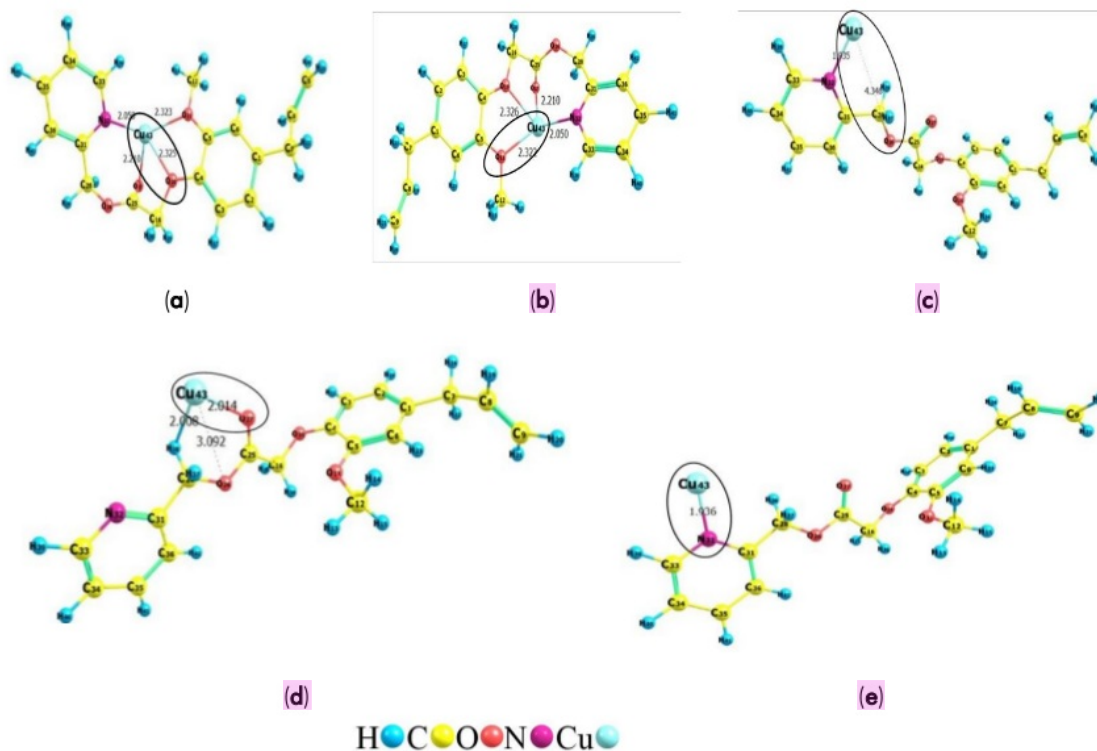


Figure 7. Geometry optimization of pyridine methyl eugenoxo acetate (PMEOA) that has interacted with Cu^{2+} in positions (a) PMEOA O_{10} atom $\dots\text{Cu}^{2+}$ (b) PMEOA O_{11} atom $\dots\text{Cu}^{2+}$ (c) PMEOA O_{26} atom $\dots\text{Cu}^{2+}$ (d) PMEOA O_{27} atom $\dots\text{Cu}^{2+}$ (e) PMEOA N_{32} atom $\dots\text{Cu}^{2+}$

Table 1. Bond length, angle, and energy obtained from geometry optimization of molecular interaction structure.

Complexes	Bond length	(Å)	Bond angle	Degree	Energy (kJ/mol)
Eugenol	Cu ₂₅ ...O ₁₀	2.04774	C ₄ -O ₁₀ ...Cu ₂₅	113.57918	-766.554
	Cu ₂₅ ...O ₁₁	2.0613	C ₅ -O ₁₁ ...Cu ₂₅	113.68029	-766.523
EOA	Cu ₃₁ ...O ₁₀	2.19375	C ₄ -O ₁₀ ...Cu ₃₁	115.13062	-879.662
	Cu ₃₁ ...O ₁₁	2.14228	C ₅ -O ₁₁ ...Cu ₃₁	122.29807	-877.986
	Cu ₃₁ ...O ₂₆	2.96157	C ₂₅ -O ₂₆ ...Cu ₃₁	69.98086	-859.391
	Cu ₃₁ ...O ₂₇	2.00613	C ₂₅ -O ₂₇ ...Cu ₃₁	120.98512	-879.661
PMEOA	Cu ₄₃ ...O ₁₀	2.32538	C ₅ -O ₁₀ ...Cu ₄₃	88.73277	-1042.046
	Cu ₄₃ ...O ₁₁	2.32166	C ₅ -O ₁₁ ...Cu ₄₃	122.84923	-1042.044
	Cu ₄₃ ...O ₂₆	4.34555	C ₂₅ -O ₂₆ ...Cu ₄₃	115.37284	-990.714
	Cu ₄₃ ...O ₂₇	2.0138	C ₂₅ -O ₂₇ ...Cu ₄₃	122.82326	-912.450
	Cu ₄₃ ...N ₃₂	1.935510	C ₃₁ -N ₃₂ ...Cu ₄₃	121.54048	-995.279

Table 2. Comparison of bond length, angle and dihedral results from geometry optimization of molecular structure

Molecule	Bond length	(Å)	Bond angle	Degree	Torsion Angles	Degree
Eugenol						
Optimization	O ₁₀ -C ₄	1.34861	C ₃ -C ₄ -O ₁₀	120.1614	C ₂ -C ₃ -C ₄ -O ₁₀	179.9665
	O ₁₁ -C ₅	1.35878	C ₄ -C ₅ -O ₁₁	114.1238	C ₃ -C ₄ -C ₅ -O ₁₁	179.9422
Interaction						
Configuration 1	O ₁₀ -C ₄	1.36927	C ₃ -C ₄ -O ₁₀	122.3264	C ₂ -C ₃ -C ₄ -O ₁₀	-179.273
Configuration 2	O ₁₁ -C ₅	1.36581	C ₄ -C ₅ -O ₁₁	116.2912	C ₃ -C ₄ -C ₅ -O ₁₁	-179.408
EOA						
Optimization	O ₁₀ -C ₄	1.36849	C ₃ -C ₄ -O ₁₀	120.0898	C ₂ -C ₃ -C ₄ -O ₁₀	-176.416
	O ₁₁ -C ₅	1.35068	C ₄ -C ₅ -O ₁₁	115.9893	C ₃ -C ₄ -C ₅ -O ₁₁	179.6043
	O ₂₆ -C ₂₅	1.33661	C ₁₆ -C ₂₅ -O ₂₇	113.7281	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	179.4115
	O ₂₇ -C ₂₅	1.17834	C ₁₆ -C ₂₅ -O ₂₇	125.3131	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	-0.00411
Interaction						
Configuration 1	O ₁₀ -C ₄	1.35951	C ₃ -C ₄ -O ₁₀	124.1649	C ₂ -C ₃ -C ₄ -O ₁₀	179.0462
Configuration 2	O ₁₁ -C ₅	1.32628	C ₄ -C ₅ -O ₁₁	114.8564	C ₃ -C ₄ -C ₅ -O ₁₁	-179.701
Configuration 3	O ₂₆ -C ₂₅	1.30246	C ₁₆ -C ₂₅ -O ₂₇	116.9226	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	-179.976
Configuration 4	O ₂₇ -C ₂₅	1.19695	C ₁₆ -C ₂₅ -O ₂₇	121.7505	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	-6.13855
PMEOA						
Optimization	O ₁₀ -C ₄	1.36678	C ₃ -C ₄ -O ₁₀	120.0927	C ₂ -C ₃ -C ₄ -O ₁₀	-176.327
	O ₁₁ -C ₅	1.34967	C ₄ -C ₅ -O ₁₁	115.9279	C ₃ -C ₄ -C ₅ -O ₁₁	-179.991
	O ₂₆ -C ₂₅	1.33915	C ₁₆ -C ₂₅ -O ₂₇	117.1841	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	178.6205
	O ₂₇ -C ₂₅	1.18047	C ₁₆ -C ₂₅ -O ₂₇	123.6502	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	0,55763
	N ₃₂ -C ₃₁	1.32213	C ₂₈ -C ₃₁ -N ₃₂	114.7156	O ₂₆ -C ₂₈ -C ₃₁ -N ₃₂	-159,967
Interaction						
Configuration 1	O ₁₀ -C ₄	1.30288	C ₃ -C ₄ -O ₁₀	126.0435	C ₂ -C ₃ -C ₄ -O ₁₀	-179.452
Configuration 2	O ₁₁ -C ₅	1.32027	C ₄ -C ₅ -O ₁₁	114.2208	C ₃ -C ₄ -C ₅ -O ₁₁	179.0307
Configuration 3	O ₂₆ -C ₂₅	1.32519	C ₁₆ -C ₂₅ -O ₂₇	110.3717	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	163.4247
Configuration 4	O ₂₇ -C ₂₅	1.20661	C ₁₆ -C ₂₅ -O ₂₇	124.4902	O ₁₀ -C ₁₆ -C ₂₅ -O ₂₇	-3.36745
Configuration 5	N ₃₂ -C ₃₁	1.33613	C ₂₈ -C ₃₁ -N ₃₂	113.6548	O ₂₆ -C ₂₈ -C ₃₁ -N ₃₂	-166.615

Tabel 3. Energy Optimization of molecular structure with interactions of molecules and without molecular interactions

Molecule	Energy (kJ/mol)					Optimization
	Configuration 1	Configuration 2	Configuration 3	Configuration 4	Configuration 5	
Eugenol	-5706420.41	-5706420.379				-5705653.856
EOA	-6301540.971	-6301539.295	-6301520.701	-6301540.971		-6300661.31
PMEOA	-7048798.877	-7048845.643	-7048845.642	-7048794.311	-7048716.047	-7047803.598

As a result of the interaction, there is a change in the geometrical structure of the molecules. The changes can include the dihedral angle and the energy. The results of the calculations are presented in **Table 3** where the molecules that had been interacted with Cu^{2+} are more stable than the molecules that had not. This is demonstrated by the energy produced by the Cu^{2+} -interacting molecules that is lower than the molecules that have not been interacted with Cu^{2+} . In particular, the most stable molecule was the PMEOA $\text{Cu}_{43}\dots\text{O}_{10}$ molecule with the lowest energy produced compared to the other molecules is shown in **Table 3**.

CONCLUSIONS

This study has confirmed the experimental results of the extraction of Cu metal ion with eugenol and its derivatives (EOA, PMEOA) with computational studies. Experimental results of eugenol and synthesis of eugenol derivatives in the form of EOA and PMEOA were applied to extract Cu^{2+} . Empirically the PMEOA was the best in extracting Cu^{2+} exceeding eugenol and EOA proven by the percentage of Cu^{2+} extracted in PMEOA, EOA and eugenol at 78.76%, 0.62%, and 0% respectively. Experimental results are supported by computational studies in which the most negative interaction energy generated comes from the PMEOA molecule. Thus it can be concluded that PMEOA is the most stable molecule in creating interaction with Cu^{2+} .

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