

Isolation and Antibacterial Activity by *in vitro* and *in silico* Approach of 6-Deoxyjacareubin Compound from *Garcinia latissima* Miq. Fruit

Neneng Siti Silfi Ambarwati¹, Berna Elya², Amarila Malik², Yuditya Artha², Islamudin Ahmad³, Azminah Azminah⁴, Muhammad Hanafi^{5,6,*}, and Hanita Omar⁷

¹Faculty of Engineering, Universitas Negeri Jakarta, Jl. Rawamangun Muka, East Jakarta 13220, Indonesia

²Faculty of Pharmacy, Universitas Indonesia, UI Depok Campus, Depok 16424, West Java, Indonesia

³Department of Pharmaceutical Sciences, Faculty of Pharmacy, Mulawarman University, Jl. Kuaro, Gn. Kelua, Samarinda 75119, East Kalimantan, Indonesia

⁴Faculty of Pharmacy, Universitas Surabaya, Jl. Raya Kalirungkut, Surabaya 60293, East Java, Indonesia

⁵Research Centre for Chemistry-Indonesian Institute of Sciences, Kawasan PUSPIPTK Serpong, Tangerang Selatan 15314, Banten, Indonesia

⁶Faculty of Pharmacy, Pancasila University, Jl. Srengseng Sawah, Jagakarsa, South Jakarta 12640, Indonesia

⁷Chemistry Division, Centre for Foundation Studies in Science, University of Malaya, Kuala Lumpur, Malaysia

* Corresponding author:

email: hanafi124@yahoo.com

Received: February 17, 2019

Accepted: October 7, 2019

DOI: 10.22146/ijc.43641

Abstract: The previous research showed that the fraction C from active extract of *Garcinia latissima* Miq. fruit was active against *Bacillus subtilis*. This study aims to isolate and identify the active compound as an antibacterial agent from the fraction C. Fraction C was purified by recrystallization using chloroform and n-hexane solvents and then isolated using preparative-thin layer chromatography-silica gel 60 GF₂₅₄ to give a yellow compound. The antibacterial activity was determined using microdilution with thiazolyl blue tetrazolium bromide indicator against *B. subtilis* American Type Culture Collection 6633. The isolate was identified using UV-Vis, IR, MS, Proton Nuclear Magnetic Resonance (¹H-NMR) and carbon NMR (¹³C-NMR), and NMR-2D techniques including HMQC and HMBC. Based on the spectroscopic analysis and literature review, the compound was identified as 6-deoxyjacareubin, which is a new compound from *Garcinia latissima* Miq. The 6-deoxyjacareubin showed antibacterial activity with MIC value of 156.25 ppm and was categorized as a weak antibacterial agent because the MIC value was more than 100 ppm. According to *in silico* approach to the docking study, 6-deoxyjacareubin showed similar hydrophobic interaction with several amino acid residues including C2565, C2589, G2484, U2590, and U5588 between a native ligand.

Keywords: 6-deoxyjacareubin; antibacterial; *Bacillus subtilis*; *Garcinia latissima* Miq.

■ INTRODUCTION

Humans have a dependence on herbal medicines in treating various diseases. Herbal medicines have been used long before the discovery of modern synthetic drugs, as traditional medicines that have always been a part of human traditions and cultures [1]. The sources of traditional medicine can be obtained from plants, including abundant native Indonesian plants [2].

Therefore, these plants need to be investigated further so that native Indonesian plants can continue to be main sources of traditional medicine [2].

One of the important part of medicine for human is their antimicrobial activity [3]. The use of antibiotics has reached an alarming level of resistance. The emergence of toxicity and the reduced effectiveness of using synthetic drugs are other problems that must be

resolved [4]. Therefore, it is necessary to do research to look for compounds from natural ingredients that have antibacterial activity [4]. This study is to test the antimicrobial activity on native Indonesian plants. The qualitative methods of the antimicrobial test include bioautography and diffusion methods, while the quantitative method of antimicrobial test is performed by the dilution method so that the minimum inhibitory concentration value can be obtained [5].

Garcinia latissima Miq. (Clusiaceae) is a plant that grows in tropical and subtropical regions. The fruit of this plant is sweet, sour and rich in nutrition. A previous study showed that 2% of the *G. latissima* Miq. fruit ethyl acetate extract in dimethyl sulfoxide (DMSO) gave inhibition zone diameter against *B. subtilis* of 9.62 mm and the minimum inhibitory concentration (MIC) against *B. subtilis* of the extract was 2500 ppm [6]. The extract was fractionated by column chromatography. Fraction C had the highest activity from 11 fractions (FA-K). The result of the activity test against *B. subtilis* from the previous study of the fraction C 2% in DMSO provided inhibition zone diameter of 9.46 mm and MIC of 1250 ppm [7].

In this study, isolation of fraction C was performed as well as antibacterial test of the isolated result. The presence of pharmacophore groups in the active compound can be used as antibacterial treatment against *B. subtilis* [8]. The positive control that was used as an antibacterial agent against *B. subtilis* was erythromycin that works by inhibiting protein synthesis [9]. The mechanism of erythromycin in the system was observed by the formation of a peptide bond with a ribosomal 50S subunit of bacteria (1:1) thereby inhibiting peptidyl transferase activity present in the 23S rRNA in the 50S subunit [10]. rRNA 23S consists of six domains, two of which are peptidyl transferase sites that are domains V and II connected by 5S rRNA [11]. Erythromycin binds specifically to adenine 2058 in domain V to inhibit the synthesis of a nascent 50S ribosomal subunit from *B. subtilis* [11]. This causes the distribution mRNA to be inhibited and affects the binding of peptidyl tRNA [10]. Molecular docking studies can further find more effective antibacterial agents [8].

6-Deoxyjacareubin isolated from *Calophyllum zeylanicum*, and *Kielmeyera speciosa* woods (Guttiferae) was reported to have antimicrobial activity [12]. 6-Deoxyjacareubin compound has been reported to be isolated from *Calophyllum inophyllum* L. [13]. *Calophyllum inophyllum* stem bark methanol extract acts as an antibacterial agent against *Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Staphylococcus epidermidis* at 25 µg/mL concentration and against *Bacillus licheniformis*, *Bacillus subtilis*, *Escherichia coli* and *Klebsiella pneumoniae* at 50 µg/mL concentration [14]. Oil from *C. inophyllum* L. has an antibacterial activity against Gram negative bacteria [15].

■ EXPERIMENTAL SECTION

Materials

The fruits of *G. latissima* Miq. were obtained from Bogor Botanical Gardens and has been identified by the center for plant conservation Bogor Botanical Garden, Indonesian Institute of Sciences (LIPI).

The chemical materials used in this study were *n*-hexane, ethyl acetate, methanol, distilled water, glacial acetic acid, thin layer chromatography-silica gel 60 GF₂₅₄, silica gel G₆₀, H₂SO₄, AlCl₃, nutrient agar, cetrinide, Thiazolyl blue tetrazolium bromide, p.a. solvents such as *n*-hexane, ethyl acetate, ethanol, chloroform, dichloromethane, methanol, and acetone.

n-Hexane, ethyl acetate, methanol, and distilled water were from Brataco Chemica, the p.a. solvents were purchased from Smart Laboratory, glacial acetic acid was purchased from Merck, thin layer chromatography-silica gel 60 GF₂₅₄, silica gel G₆₀, H₂SO₄, AlCl₃, nutrient agar, and cetrinide was purchased from Merck, while Thiazolyl blue tetrazolium bromide was purchased from BBI Life Sciences.

Instrumentation

The equipment used in the study were a rotary evaporator, column chromatography equipment, thin layer chromatography equipment, vials and bottles, micro pipet, UV-Vis spectrophotometer, analytical balance, glasswares, CAMAG UV cabinet 4, electric stove,

Memmert oven, refrigerator, infra-red spectrophotometer, nuclear magnetic resonance spectroscopy, High Performance Liquid Chromatography–Mass Spectrometry–Mass Spectrometry, microplate 96-well and Memmert incubator.

Procedure

Extraction, fractionation, and isolation processes

The extraction process of *G. latissima* fruits (8.9 kg) by successive maceration (by three solvents: *n*-hexane, ethyl acetate, and methanol) was performed according to the study by Ambarwati et al. [6]. Moreover, the *G. latissima* fruits ethyl acetate extract (157 g) was fractionated. The fractionation was conducted using column chromatography according to the study by Ambarwati et al. [7] and resulted in 11 fractions (A-K).

The material used for the isolation was the fraction C of ethyl acetate extract of *G. latissima* Miq. fruits (1.53 g). Fraction C was separated on silica gel column chromatography (CC) (305 mm × 23 mm i.d) with *n*-hexane/ethyl acetate (100:0–0:100, v/v) as eluents and then purified by recrystallization and thin layer chromatography-silica gel. The recrystallization of fraction C was processed by modifying the non-polar solvent (hexanes) and the semi-polar solvent (ethyl acetate). And then, fraction C was purified further using preparative thin-layer chromatography (*p*-TLC) method. From the purification, 6-deoxyjacareubin was obtained and then identified using thin-layer chromatography with *n*-hexane-chloroform (1:4, v/v) as the mobile system. The retention factor (*R_f*) value of the isolate obtained from thin-layer chromatography with *n*-hexane-chloroform was 0.4.

Antibacterial activity

The antibacterial activity of the compound was evaluated against *B. subtilis* ATCC 6633 which was taken from the laboratory of Microbiology, Faculty of Pharmacy, Universitas Indonesia. The bacterial cultures were developed by selective nutrient agar at 37 °C for 24 h [1]. The nutrient broth was used for the preparation of inoculum of the bacteria, and nutrient agar was used for the screening method. The antibacterial activity test against *B. subtilis* was carried out by microdilution

method using yellow indicator tetrazolium salt (MTT) so that the MIC value (in triplicates) is obtained.

In silico molecular study

Crystal structure of peptidyl transferase was downloaded from the RCSB protein data bank complexed with erythromycin (PDB ID: 1JZY) [16]. The macromolecule enzyme was reduced by removing several of the nonessential residues to minimize the macromolecule size. Docking method was validated by re-docking the co-crystallized ligand (erythromycin) into the same active site of the enzyme using AutoDock Tools, and the results were determined by values of Root Mean Square Deviation (RMSD). Subsequently, the ligand (6-deoxyjacareubin) was optimized by adding charge using Antechamber and docked into the same active site. Gasteiger charge was added to both ligands; free binding energy values were calculated and analyzed. The ligand-residue interaction was visualized using LigPlot to observe involved residue which contributed to the values of binding affinity.

RESULTS AND DISCUSSION

The 6-deoxyjacareubin compound obtained was observed as yellow needles crystals (16.8 mg) which were obtained from chloroform solution. The molecular formula was determined to be C₁₈H₁₄O₅ from its quasi-molecular ion peak at *m/z* 311.43 [M+H]⁺ (molecular-weight or exact mass was calculated 310.0841) in the Liquid Chromatography–Mass Spectrometry spectra which are shown in Fig. 1.

The results of the UV isolate spectrum (Fig. 2) showed that the isolate using chloroform solvent, had the maximum λ absorption, at 308 and 329 nm. The maximum wavelength (329 nm) indicates that the compound contained a conjugated unsaturated ketone. The unsaturated conjugated bond is a single and double bond that alternate each other [17]. The maximum wavelength of 308 nm indicates the presence of a substituted benzene ring, the xanthone framework [18].

The hydroxyl group (–OH) was detected in the IR spectrum at 3425 cm⁻¹ (shown in Fig. 3). The absorption bands at 2900 and 2800 cm⁻¹ indicate the vibration of the

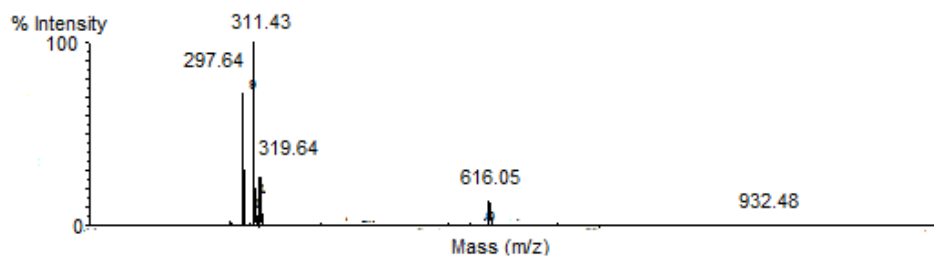


Fig 1. The Liquid chromatography–mass spectrometry spectra of compound 1

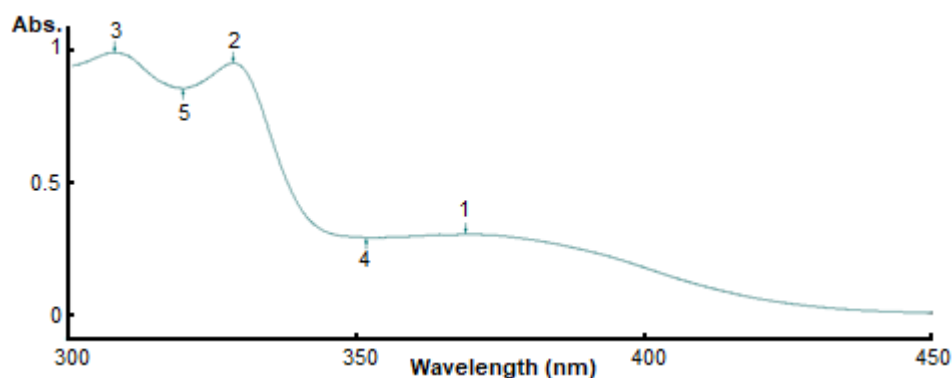


Fig 2. The UV spectrum of compound 1

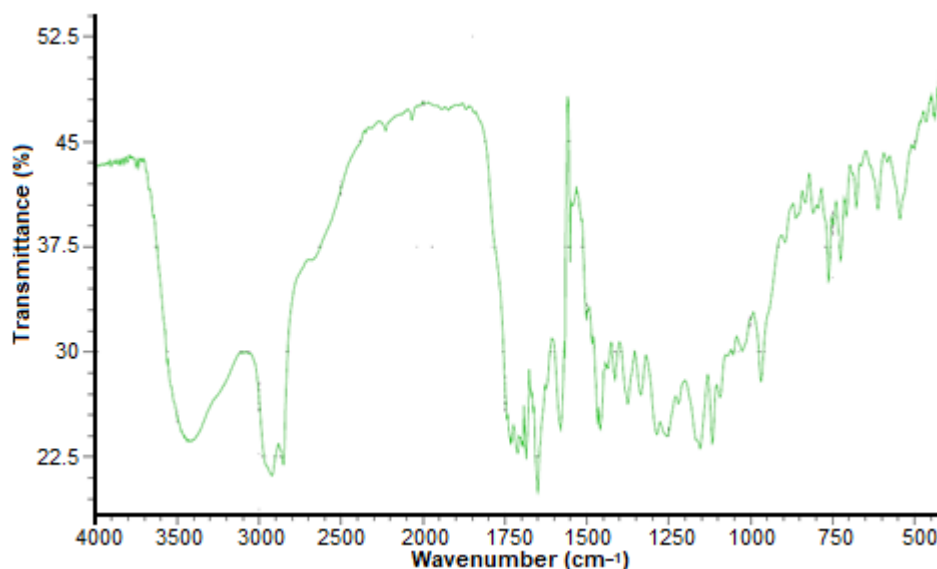


Fig 3. The IR spectrum of compound 1

CH (CH, CH₂, CH₃). The presence of an absorption band at 1680 cm⁻¹ indicates the vibration of the phenyl group [18]. From these infra-red spectra data, it is estimated that these compounds contain hydroxyl groups, phenyl groups, and CH, CH₂, or CH₃ groups.

The ¹H-NMR spectrum showed a specific peak in the aliphatic region at δ_H 1–2 ppm (Fig. 4). There is also a peak that characterizes a xanthone derivative of a dimethyl

group present at δ_H 1.49 (s, 6H) and two doublet protons (as a chromene) at δ_H 5.78 (d, *J* = 10.4 Hz) and δ_H 7.06 (d, *J* = 10.4 Hz) [19]. A coupling constant *J* value (in Hz) in NMR proton provides information in measuring the interaction of proton pairs. Protons in an ortho relationship show large coupling (8–12 Hz, but normally about 10); protons with a meta relationship show a small coupling (2–6 Hz). Furthermore, there is one singlet

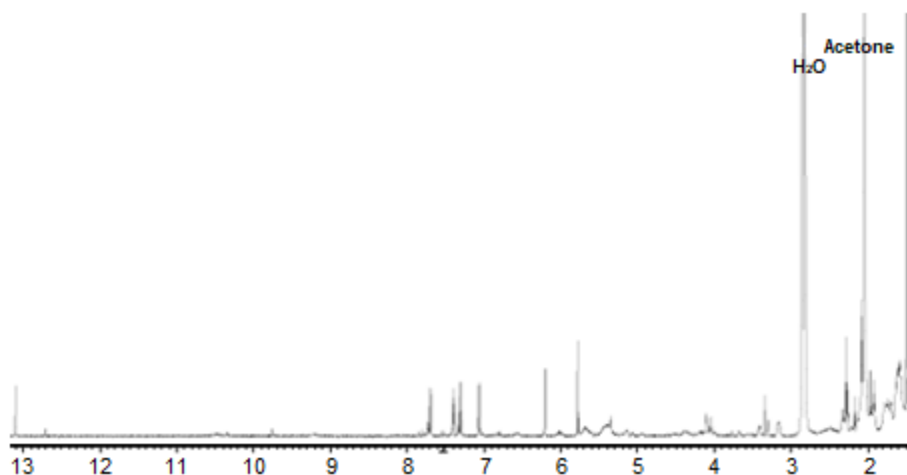


Fig 4. The spectrum of H-NMR

Table 1. ¹H-NMR and ¹³C-NMR data compound 1 compared with 6-deoxyjacareubin

No	Compound 1 (in acetone-d6)		6-Deoxyjacareubin (in acetone-d6) [19]	
	δ ¹³ C-NMR	δ ¹ H-NMR (m, J in Hz)	δ ¹³ C-NMR	δ ¹ H-NMR (m, J in Hz)
1	116.0	7.0 (dd, 8.4; 2.0)	116.7	7.66 (dd, 7.8, 1.6)
1a	122.6	-	-	-
2	121.9	7.31 (t, 8, 4)	122.6	7.27 (t, 7.8)
3	122.6	7.39 (dd, 8.4, 2.0)	122.6	7.35 (dd, 7.8, 1.6)
4	146.8	-	144.3	-
4a	147.5	-	-	-
5	99.9	6.21 (s)	-	6.40 (s)
5a	164.2	-	-	-
6	153.0	-	159.5	-
7	104.5	-	106.3	-
8	162.3	13.1 (s)	162.7	13.33 (s)
9	182.5	-	-	-
9a	102.7	-	-	-
10	116.5	7.06 (d, 10.4)	-	6.69 (d, 10.1)
11	128.4	5.75 (d, 10.4)	-	5.76 (d, 10.2)
12	78.3	-	-	-
13, 14	28.2	1.50 (6H, s)	-	1.48 (6H, s)

proton at δ_H 6.21 (s) and aromatics with an ABC system appearing at δ_H 7.39 (dd); 7.31 (t) and 7.71 (dd). The presence of particular groups in the highly downfield region of δ_H 13.10 (s), is also a characteristic that this compound is thought to be a xanthone derivative [19]. The ¹H-NMR and ¹³C-NMR data compound were compared with 6-deoxyjacareubin (chromenoxantone group) [20]; see Table 1. We concluded this structure to be as described in Fig. 5.

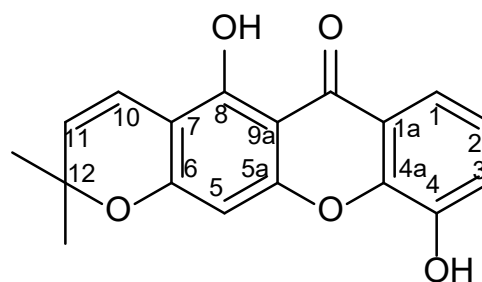


Fig 5. The structure of compound 1

Table 2. Calculated estimated binding free energy and inhibition constant in docking of 6-deoxyjacareubin to erythromycin

No	Compound	Binding free energy		Inhibition constant	
1	Erythromycin (redocking)	RMSD 2.00 Å -5.75 kcal/mol		RMSD 2.00 Å 61.27 μM	
2	6-Deoxyjacareubin	Best rank -5.66 kcal/mol	Best cluster 6/10 = -5.66 kcal/mol	Best rank 70.87 μM	Best cluster 70.87 μM

two benzenes with O atoms and ketones, have lipophilic properties and some of these compounds have been studied as anti-*B. subtilis* [26].

The isolate with a MIC value of 156.25 ppm shows that anti-bacterial activity against *B. subtilis* is low since the value of MIC > 100 ppm [27]. This also corresponds with the fraction C activity from the fruit's ethyl acetate extract that has a value of 1250 ppm. The value from fraction C shows that it has a low activity against *B. subtilis* since the value of MIC > 625 ppm [27].

In Silico

The ligand stability is defined by RMSD value obtained from docking studies. Ligand stability is determined by RMSD value which describes the different coordinates to the best docking score. In this study, the ligand exhibited RMSD value of below 2.00 Å. Thus it shows that by using reduced macromolecule, the ligand was able to maintain the coordinate stability by showing similar coordinates within 10 runs of docking. Further molecular dynamic study is required to understand the properties of reduced macromolecule [28].

The affinity and inhibition constant (k_i) were -5.75 kcal/mol and 61.27 μM, respectively. 6-Deoxyjacareubin resulted in lower affinity compared to the cocrystal structure of erythromycin with binding energy and inhibition constant of -5.66 kcal/mol and 70.87 μM, respectively. Docking results of 6-deoxyjacareubin showed interaction with several residues in concordance to the residues bonded with erythromycin. These residues included U2588, C2589, G2484, and U2590, indicating similar activity of 6-deoxyjacareubin with erythromycin. The table of calculated estimated binding free energy and inhibition constant in the docking of 6-deoxyjacareubin to

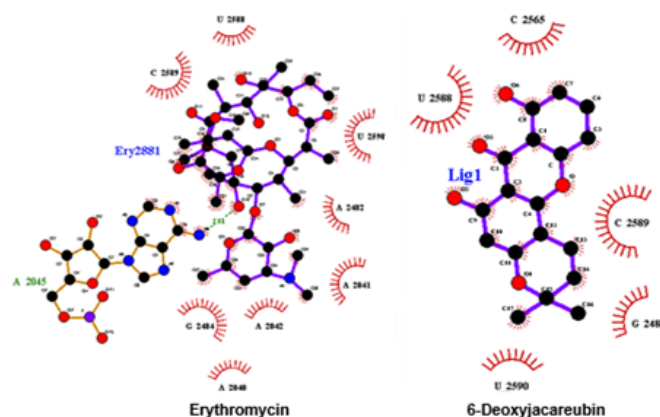


Fig 8. The interaction between erythromycin and 6-deoxyjacareubin with amino acids on the A2042 PDB receptor using the LigPlot program was illustrated

erythromycin can be seen in Table 2 [17].

Erythromycin involved hydrogen bonding with A2042 which was not shown on deoxyjacareubin. The hydrogen bonding might have contributed to erythromycin affinity which was slightly higher than deoxyjacareubin. Both ligands exhibited similar hydrophobic interaction with several residues. The interaction between erythromycin and 6-deoxyjacareubin with amino acids on the A2042 PDB receptor using the LigPlot program is illustrated in Fig. 8.

CONCLUSION

Deoxyjacareubin compounds were isolated from the ethyl acetate extract of *G. latissima* Miq. fruit, and acted as an antibacterial agent against *B. subtilis* with a MIC value of 156.25 ppm. According to the docking study, 6-deoxyjacareubin showed similar hydrophobic interaction with several amino acid residues (including C2565, C2589, G2484, U2590, and U5588) between a native ligand.

■ ACKNOWLEDGMENTS

The research was supported by the Ministry of Research, Technology and Higher Education of the Republic of Indonesia with the contract number: 1/SP2H/DRPM/LPPM-UNJ/III/2019.

■ REFERENCES

- [1] Kochuthressia, K.P., Britto, S.J., Jaseentha, M.O., and Raphael, R., 2012, In vitro antimicrobial evaluation of *Kaempferia galanga* L. rhizome extract, *Am. J. Biotechnol. Mol. Sci.*, 2 (1), 1–5.
- [2] Sholikhah, E.N., 2016, Indonesian medicinal plants as sources of secondary metabolites for pharmaceutical industry, *J. Med. Sci.*, 48 (4), 226–239.
- [3] Nascimento, G.G.F., Locatelli, J., Freitas, P.C., and Silva, G.L., 2000, Antibacterial activity of plant extracts and phytochemicals on antibiotic-resistant bacteria, *Braz. J. Microbiol.*, 31 (4), 247–256.
- [4] Dzotam, J.K., and Kuete, V., 2017, Antibacterial and antibiotic-modifying activity of methanol extracts from six Cameroonian food plants against multidrug-resistant enteric bacteria, *BioMed Res. Int.*, 2017, 1583510.
- [5] Valgas, C., de Souza, S.M., Smânia, E.F.A., and Smania, Jr.A., 2007, Screening methods to determine antibacterial activity of natural products, *Braz. J. Microbiol.*, 38 (2), 369–380.
- [6] Ambarwati, N.S.S., Elya, B., Malik, A., and Hanafi, M., 2017, Phytochemical and antimicrobial studies on *Garcinia latissima* Miq. fruits extract, *Asian J. Pharm. Clin. Res.*, 10 (7), 230–232.
- [7] Ambarwati, N.S.S., Malik, A., Listari, A.T., Nirwana, Elya, B., and Hanafi, M., 2017, Antibacterial activity of fractions of ethyl acetate extract of *Garcinia latissima* Miq. fruits, *Asian J. Pharm. Clin. Res.*, 10 (17), 81–84.
- [8] Bhakiaraj, D., Elavarasan, T., and Gopalakrishnan, M., 2014, Synthesis, spectral analysis, antimicrobial evaluation and molecular docking studies of some novel 3,5-dichloro-2,6-diarylpiperidin-4-ones, *Der Pharma Chem.*, 6 (5), 243–250.
- [9] Lin, J.T., Connelly, M.B., Amolo, C., Otani, S., and Yaver, D.S., 2005, Global transcriptional response of *Bacillus subtilis* to treatment with subinhibitory concentrations of antibiotics that inhibit protein synthesis, *Antimicrob. Agents Chemother.*, 49 (5), 1915–1926.
- [10] Champney, W.S., and Burdine, R., 1995, Macrolide antibiotics inhibit 50S ribosomal subunit assembly in *Bacillus subtilis* and *Staphylococcus aureus*, *Antimicrob. Agents Chemother.*, 39 (9), 2141–2144.
- [11] Pechère, J.C., and Kaplan, E.L., 2004, *Streptococcal Pharyngitis: Optimal Management*, Karger Medical and Scientific Publishers, Basel, Switzerland.
- [12] Harborne, J.B., Baxter, H., and Moss, G.P., 1999, *Phytochemical Dictionary A Handbook of Bioactive Compounds from Plants*, 2nd Ed., CRC Press, Boca Raton, Florida.
- [13] Iinuma, M., Tosa, H., Tanaka, T., and Yonemori, S., 1994, Two new xanthenes in the underground part of *Calophyllum inophyllum*, *Heterocycles*, 37 (2), 833–838.
- [14] Oo, W.M., 2018, Pharmacological properties of *Calophyllum inophyllum* – Updated review, *Int. J. Photochem. Photobiol.*, 2 (1), 28–32.
- [15] Lim, T.K., 2012, *Edible Medicinal and Non-Medicinal Plants*, Springer, Netherlands.
- [16] Schlünzen, F., Zarivach, R., Harms, J., Bashan, A., Tocilj, A., Albrecht, R., Yonath, A., and Franceschi, F., 2001, Structural basis for the interaction of antibiotics with the peptidyl transferase centre in eubacteria, *Nature*, 413 (6858), 814–821.
- [17] Dewick, P.M., 2006, *Essentials of Organic Chemistry for Students of Pharmacy, Medicinal Chemistry and Biological Chemistry*, 1st Ed., Wiley, Hoboken, New Jersey.
- [18] Wu, Y.P., Zhao, W., Xia, Z.Y., Kong, G.H., Lu, X.P., Hu, Q.F., and Gao, X.M., 2013, Three novel xanthenes from *Garcinia paucinervis* and their anti-TMV activity, *Molecules*, 18 (8), 9663–9669.
- [19] Yi, B., Hu, L., Mei, W., Zhou, K., Wang, H., Luo, Y., Wei, X., and Dai, H., 2010, Antioxidant phenolic compounds of cassava (*Manihot esculenta*) from

- Hainan, *Molecules*, 16 (12), 10157–10167.
- [20] Hostettmann, K., Marston, A., and Hostettmann, M., 1998, *Preparative Chromatography Techniques Applications in Natural Product Isolation*, 2nd Ed., Springer-Verlag, Berlin Heidelberg.
- [21] Kurniawati, P.T., Soetjipto, H., and Limantara, L., 2007, Antioxidant and antibacterial activities of bixin pigment from annatto (*Bixa orellana* L.) seeds, *Indones. J. Chem.*, 7 (1), 88–92.
- [22] Su, P.W., Yang, C.H., Yang, J.F., Su, P.Y., and Chuang, L.Y., 2015, Antibacterial activities and antibacterial mechanism of *Polygonum cuspidatum* extracts against nosocomial drug-resistant pathogens, *Molecules*, 20 (6), 11119–11130.
- [23] Gupta, R., Beg, Q.K., and Lorenz, P., 2002, Bacterial alkaline proteases: Molecular approaches and industrial applications, *Appl. Microbiol. Biotechnol.*, 59 (1), 15–32.
- [24] Hostettmann, K., and Hostettmann, M., 1989, “Xanthones” in *Methods in Plant Biochemistry*, vol. 1, Eds. Harborne, J.B., Academic Press, London, 493–508.
- [25] Narasimhan, S., Maheshwaran, S., Abu-Yousef, I.A., Majdalawieh, A.F., Rethavathi, J., Das, P.E., and Poltronieri, P., 2017, Anti-bacterial and anti-fungal activity of xanthones obtained via semi-synthetic modification of α -mangostin from *Garcinia mangostana*, *Molecules*, 22 (2), 275.
- [26] Fukai, T., Oku, Y., Hou, A.J., Yonekawa, M., and Terada, S., 2004, Antimicrobial activity of hydrophobic xanthones from *Cudrania cochinchinensis* against *Bacillus subtilis* and methicillin-resistant *Staphylococcus aureus*, *Chem. Biodivers.*, 1 (9), 1385–1390.
- [27] Awouafack, M.D., McGaw, L.J., Gottfried, S., Mbouangouere, R., Tane, P., Spiteller, M., and Eloff, J.N., 2013, Antimicrobial activity and cytotoxicity of the ethanol extract, fractions and eight compounds isolated from *Eriosema robustum* (Fabaceae), *BMC Complem. Altern. Med.*, 13, 289.
- [28] Liu, K., and Kokubo, H., 2017, Exploring the stability of ligand binding modes to proteins by molecular dynamics simulations: A cross-docking study, *J. Chem. Inf. Model.*, 57 (10), 2514–2522.

Vol 20, No 4 (2020)

Accredited by RISTEK-BRIN No.: 85/M/KPT/2020 (April 1, 2020)

ISSN: 1411-9420 (print), 2460-1578 (online)

Indonesian Journal of Chemistry

Vol. 20, No. 4, August 2020

The image displays two ball-and-stick molecular models. The left model is labeled 'Erythronycin' and shows a complex polycyclic structure with various atoms (black, red, blue, green) and several curved arrows indicating bond lengths and angles. The right model is labeled '4-Benzoylaminamide' and shows a simpler structure with a benzene ring and an amide group, also with curved arrows indicating bond lengths and angles.

Accredited by RISTEK-BRIN
No. 85/M/KPT/2020

Indones. J. Chem. Vol. 20 No. 4 PP 729-966 Yogyakarta August 2020 ISSN 1411-9420 (print) 2460-1578 (online)

Ads by Google

Stop seeing this ad Why this ad?

Indonesian Journal of Chemistry

COUNTRY

Indonesia

 Universities and research institutions in Indonesia

SUBJECT AREA AND CATEGORY

Chemistry
Chemistry (miscellaneous)

PUBLISHER

Gadjah Mada University

 Gadjah Mada University in Scimago Institutions Rankings

H-INDEX

14

PUBLICATION TYPE

Journals

ISSN

14119420

COVERAGE

2010, 2012-2020

INFORMATION

[Homepage](#)
[How to publish in this journal](#)
nuryono_mipa@ugm.ac.id

Ads by Google

Stop seeing this ad Why this ad?

SCOPE

Indonesian Journal of Chemistry is a peer-reviewed, open access journal that publishes original research articles, review articles, as well as short communication in all areas of chemistry, including educational chemistry, applied chemistry, and chemical engineering.

 Join the conversation about this journal

Hindawi Open Access Publishing

Our Journals are Peer-Reviewed & Open Access. Publish With Us & Reach a Wider Audience.

Hindawi

Open

Hindawi Open Access Publishing

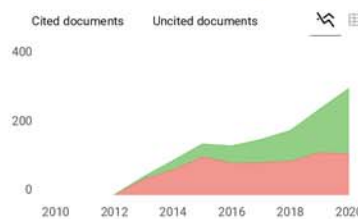
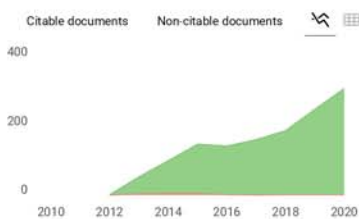
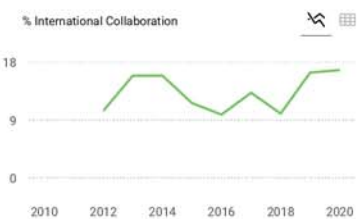
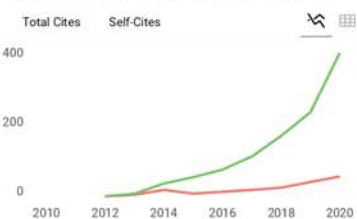
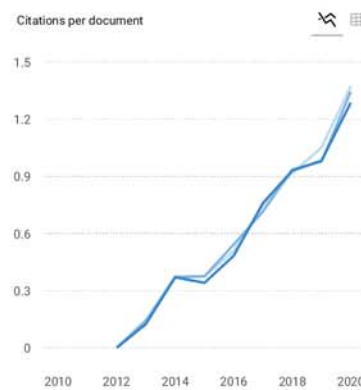
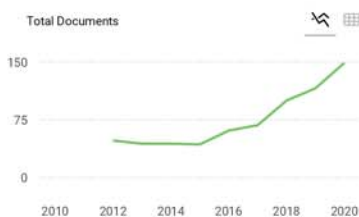
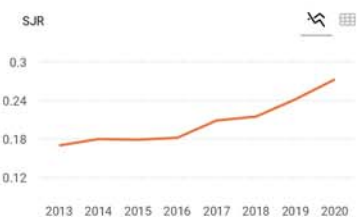
Our Journals are Peer-Reviewed & Open Access. Publish With Us & Reach a Wider Audience.

Hindawi Open

FIND SIMILAR JOURNALS

options

- | | | | | |
|---|--|---|---|--|
| <p>1
Journal of Chemistry
USA</p> <p>68%
similarity</p> | <p>2
Research Journal of Chemistry and Environment
IND</p> <p>65%
similarity</p> | <p>3
Malaysian Journal of Analytical Sciences
MYS</p> <p>61%
similarity</p> | <p>4
Arabian Journal of Chemistry
SAU</p> <p>56%
similarity</p> | <p>5
Journal of the Chemical Society of Pakistan
PAK</p> <p>54%
similarity</p> |
|---|--|---|---|--|



Indonesian Journal of Chemistry

Q3 Chemistry (miscellaneous) best quartile

SJR 2020 **0.27**

powered by scimagojr.com

Show this widget in your own website

Just copy the code below and paste within your html code:

```
<a href="https://www.scimagojr.com" style="display: inline-block; width: 100px; height: 15px; background-color: #f0f0f0; border: 1px solid #ccc;">
```

SCImago Graphica

Explore, visually communicate and make sense of data with our **new free tool**.

Get it





Source details

Indonesian Journal of Chemistry

Open Access ⓘ

Scopus coverage years: 2010, from 2012 to Present

Publisher: Gadjah Mada University

ISSN: 1411-9420

Subject area: Chemistry: General Chemistry

Source type: Journal

CiteScore 2020

1.5



SJR 2020

0.273



SNIP 2020

0.996



[View all documents >](#)

[Set document alert](#)

[Save to source list](#) [Source Homepage](#)

[CiteScore](#) [CiteScore rank & trend](#) [Scopus content coverage](#)

i Improved CiteScore methodology



CiteScore 2020 counts the citations received in 2017-2020 to articles, reviews, conference papers, book chapters and data papers published in 2017-2020, and divides this by the number of publications published in 2017-2020. [Learn more >](#)

CiteScore 2020 ▼

$$1.5 = \frac{655 \text{ Citations 2017 - 2020}}{431 \text{ Documents 2017 - 2020}}$$

Calculated on 05 May, 2021

CiteScoreTracker 2021 ⓘ

$$1.6 = \frac{694 \text{ Citations to date}}{437 \text{ Documents to date}}$$

Last updated on 04 August, 2021 • Updated monthly

CiteScore rank 2020 ⓘ

Category	Rank	Percentile
Chemistry		
General Chemistry	#248/398	37th

[View CiteScore methodology >](#) [CiteScore FAQ >](#) [Add CiteScore to your site ↗](#)

About Scopus

[What is Scopus](#)
[Content coverage](#)
[Scopus blog](#)
[Scopus API](#)
[Privacy matters](#)

Language

[日本語に切り替える](#)
[切换到简体中文](#)
[切换到繁體中文](#)
[Русский язык](#)

Customer Service

[Help](#)
[Contact us](#)

ELSEVIER

[Terms and conditions ↗](#) [Privacy policy ↗](#)

Copyright © Elsevier B.V. All rights reserved. Scopus® is a registered trademark of Elsevier B.V.

We use cookies to help provide and enhance our service and tailor content. By continuing, you agree to the use of cookies.

 RELX

Editorial Team

Editor-in-Chief

Nuryono Nuryono, Laboratory of Inorganic Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Managing Editor

Dwi Siswanta, Laboratory of Analytical Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Editorial Board

Dr. Hendrik Oktendy Lintang, Indonesia

Dr. Charles Edwin Raja Gabriel, University of Notre Dame, Notre Dame, Indiana, United States

Assoc. Prof. Dr. Roswanira Abdul Wahab, Department of Chemistry, Universiti Teknologi Malaysia, Malaysia

Mudasir Mudasir, Laboratory of Analytical Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Hideaki Hisamoto, Department of Applied Chemistry, Osaka Prefecture University, Japan

Prof. Joe da Costa, Department of Chemical Engineering, University of Queensland, Australia

Dr. Maurizio Barbieri, Department of Earth Science, Sapienza University, Italy

Ming Cai, Tongji University, China

Muhammad Idham Darussalam Mardjan, Laboratory of Organic Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Pornthep Sompornpisut, Department of Chemistry, Chulalongkorn University, Thailand

Prof. Dr. Taghreed Hashim Al-Noor, Ibn-Al-Haitham Education College /University of Baghdad, Iraq

Praveen Kumar Sharma, Department of Chemistry, Lovely Professional University, Punjab, India

Akhmad Syoufian, Laboratory of Physical Chemistry, Department of Chemistry, Universitas Gadjah Mada

Tri Joko Raharjo, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Dr. Saprizal Hadisaputra, Chemistry Education Division, Faculty of Science and Education, University of Mataram, Indonesia

Satya Candra Wibawa Sakti, Laboratory of Inorganic Chemistry, Department of Chemistry, Universitas Airlangga, Indonesia

Winifred Uduak Anake, Department of Chemistry, College of Science and Technology, Covenant University, Nigeria

Aulia Sukma Hutama, Laboratory of Physical Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Dr. Adhi Dwi Hatmanto, Universitas Gadjah Mada, Indonesia

Administration Support



















































Djoko Prihandono, Department of Chemistry, Universitas Gadjah Mada, Indonesia





























































Aulia Sukma Hutama, Laboratory of Physical Chemistry, Department of Chemistry, Universitas Gadjah Mada, Indonesia

Aulia Ratri Hapsari, Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Gadjah Mada, Indonesia

Table of Contents


Articles




Magnetic Mesoporous Silica Composite for Enhanced Preconcentration of Selected Organophosphorus Pesticides in Fruits	729-745 
 Nur Husna Zainal Abidin, Wan Nazihah Wan Ibrahim, Nor Suhaila Mohamad Hanapi, Nor'ashikin Saim	
 10.22146/ijc.42935  Abstract views : 2098  views : 1440	
Synthesis of Zinc Oxide Nanoparticles for Oil Upgrading and Wax Deposition Control: Effect of Calcination Temperature	746-754 
 Siti Nurliyana Che Mohamed Hussein, Fatin Syahirah Mohamed Fuad, Marina Ismail	
 10.22146/ijc.43317  Abstract views : 1421  views : 1211	
Adsorption-Desorption Profile of Methylene Blue Dye on Raw and Acid Activated Kaolinite	755-765 
 Nurul Ain Safiqah Md Sandollah, Sheikh Ahmad Izaddin Sheikh Mohd Ghazali, Wan Nazihah Wan Ibrahim, Ruhaida Rusmin	
 10.22146/ijc.43552  Abstract views : 1907  views : 1348	
Cytotoxic Activity of 2-O-β-glucopyranosil Cucurbitacin D from Benalu Batu (<i>Begonia</i> sp.) Growing in Morowali, Central Sulawesi	766-772 
 Muhammad Sulaiman Zubair, Walied Mohamed Alarif, Mohamed Ali Ghandourah, Syariful Anam, Ibrahim Jantan	
 10.22146/ijc.43626  Abstract views : 1944  views : 1562	
Isolation and Antibacterial Activity by <i>in vitro</i> and <i>in silico</i> Approach of 6-Deoxyjacareubin Compound from <i>Garcinia latissima</i> Miq. Fruit	773-781 
 Neneng Siti Silfi Ambarwati, Berna Elya, Amarila Malik, Yuditya Artha, Islamudin Ahmad, Azminah Azminah, Muhammad Hanafi, Hanita Omar	
 10.22146/ijc.43641  Abstract views : 1894  views : 1661	
Study of the Synthesis of Zirconia Powder from Zircon Sand obtained from Zircon Minerals Malaysia by Caustic Fusion Method	782-790 
 Istikamah Subuki, Mimi Fazzlinda Mohsin, Muhammad Hussain Ismail, Fazira Suriani Mohamed Fadzil	
 10.22146/ijc.43936  Abstract views : 1477  views : 1555	
Preparation of Ammonia Dealuminated Metakaolinite and Its Adsorption against Bixin	791-800 
 Winda Rahmalia, Jean-Francois Fabre, Thamrin Usman, Zéphirin Mouloungui	
 10.22146/ijc.44706  Abstract views : 2036  views : 1524	
Electrical and Thermal Conductivity of Cyclic Natural Rubber/Graphene Nanocomposite Prepared by Solution Mixing Technique	801-809 
 Vivi Purwandari, Saharman Gea, Basuki Wirjosentono, Agus Haryono, I Putu Mahendra, Yasir Arafat Hutapea	
 10.22146/ijc.44791  Abstract views : 2075  views : 1776	
Bioleaching Ability of Fungi Isolated from an Indonesian Sulfurous River Sediment	810-817 
 Serafica Btari Christiyani Kusumaningrum, I Wayan Warmada, Wahyu Wilopo, Endah Retnaningrum	
 10.22146/ijc.44810  Abstract views : 1652  views : 1604	
Synthesis of Soluble Novel Polyacetylenes Containing Carbamate and Eugenol Moieties	818-824 
 Erwin Abdul Rahim	
 10.22146/ijc.45603  Abstract views : 1548  views : 1018	

<p>Optimization and Characterization of Wood Vinegar Produced by <i>Shorea laevis</i> Ridl Wood Pyrolysis</p> <p> Hasan Ashari Oramahi, Tsuyoshi Yoshimura, Elvi Rusmiyanto, Kustiati Kustiati</p> <p> 10.22146/ijc.45783  Abstract views : 2078  views : 1853</p>	825-832 
<p>Preparation and Powder XRD Analysis of Tris(2,2'-bipyridine)nickel(II) Trifluoroacetate</p> <p> Kristian Handoyo Sugiyarto, Isana Supiah Yosephine Louise, Shinta Setya Wilujeng</p> <p> 10.22146/ijc.46483  Abstract views : 1520  views : 1365</p>	833-841 
<p>Carbonization of Lignin Extracted from Liquid Waste of Coconut Coir Delignification</p> <p> Widiyastuti Widiyastuti, Mahardika Fahrudin Rois, Heru Setyawan, Siti Machmudah, Diky Anggoro</p> <p> 10.22146/ijc.46484  Abstract views : 1561  views : 1218</p>	842-849 
<p>Metabolite Profile Evaluation of Indonesian Roasted Robusta Coffees by ¹H NMR Technique and Chemometrics</p> <p> Nizar Happyana, Elvira Hermawati, Yana Maolana Syah, Euis Holisotan Hakim</p> <p> 10.22146/ijc.46492  Abstract views : 1969  views : 1480</p>	850-857 
<p>Significance of Oxirane Rings in Epoxidized Palm Oil and Effects on the Coating Performance: Comparison between Epoxidized Unripe Palm Oil and Epoxidized Used Cooking Oil towards Adhesion Performance</p> <p> Nurul Hazirah Aina Hasnan, Najmiddin Yaakob, Muhammad Nadzmi Abu Kassim, Umie Amira Mohd Noh</p> <p> 10.22146/ijc.46619  Abstract views : 1747  views : 1793</p>	858-869 
<p>Fabrication of Superhydrophobic Film on the Surface of Indonesian Bamboo Timber by TiO₂ Deposition and Using Octadecyltrichlorosilane as a Surface Modifier Agent</p> <p> Diana Vanda Wellia, Wulandari Wulandari, Arifah Mustaqimah, Nurul Pratiwi, Yulia Eka Putri</p> <p> 10.22146/ijc.46740  Abstract views : 1496  views : 1209</p>	870-879 
<p>Assessment of Free and Total Cyanide Levels in the Water Environment of Shatt Al-Arab</p> <p> Zuhair Ali Abdulnabi</p> <p> 10.22146/ijc.47369  Abstract views : 1415  views : 1325</p>	880-886 
<p>High Oleic Pentaerythritol Tetraester Formation via Transesterification: Effect of Reaction Conditions</p> <p> Nor Faeqah Idrus, Robiah Yunus, Zurina Zainal Abidin, Umer Rashid, Norazah Abd Rahman</p> <p> 10.22146/ijc.47891  Abstract views : 1981  views : 2151</p>	887-898 
<p>In Silico Study on Interaction and Preliminary Toxicity Prediction of <i>Eleutherine americana</i> Components as an Antifungal and Antitoxoplasmosis Candidate</p> <p> Sophi Damayanti, Nadiyah Athifah Salim Martak, Benny Permana, Adi Suwandi, Rika Hartati, Indra Wibowo</p> <p> 10.22146/ijc.48570  Abstract views : 2244  views : 1466</p>	899-910 
<p>Cobalt Doping on Zirconium Titanate as a Potential Photocatalyst with Visible-Light-Response</p> <p> Emilya Faridatul Sulaikhah, Rian Kurniawan, Mokhammad Fajar Pradipta, Wega Trisunaryanti, Akhmad Syoufan</p> <p> 10.22146/ijc.49459  Abstract views : 1680  views : 1468</p>	911-918 
<p>Kinetic study of HTPB (Hydroxyl Terminated Polybutadiene) Synthesis Using Infrared Spectroscopy</p> <p> Heri Budi Wibowo, Widhi Cahya Dharmawan, Ratih Sanggra Murti Wibowo, Adi Yulianto</p> <p> 10.22146/ijc.49863  Abstract views : 1940  views : 4425</p>	919-928 
<p>Synthesis, Characterization, and Stability Evaluation of β-Carotene Encapsulated in Starch-Chitosan/Tripolyphosphate Matrices</p> <p> Agnes Dyah Novitasari Lestari, Dwi Siswanta, Ronny Martien, Mudasir Mudasir</p> <p> 10.22146/ijc.50449  Abstract views : 1909  views : 1420</p>	929-940 

pH Dependence on Colorimetric Detection of Hg²⁺ by Histidine-Functionalized Gold Nanoparticles


941-952 


 *Dewi Eviane, Dwi Siswanta, Sri Juari Santosa*




 [10.22146/ijc.51824](https://doi.org/10.22146/ijc.51824)  Abstract views : 1712 |  views : 1035

Short Communication

Structure-Based Design and Molecular Dynamics Simulations of Pentapeptide AEYTR as a Potential Acetylcholinesterase Inhibitor


953-959 

 *Vivitri Dewi Prasasty, Enade Perdana Istyastono*




 [10.22146/ijc.46329](https://doi.org/10.22146/ijc.46329)  Abstract views : 2048 |  views : 1409

Note

Effect of Microwave Pretreatment on Gaharu Essential Oil Using Hydrodistillation Method

960-966 

 *Nurhaslina Che Radzi, Filzah Anati Kasim*

 [10.22146/ijc.43191](https://doi.org/10.22146/ijc.43191)  Abstract views : 1316 |  views : 1235