Revealing Potency of Bioactive Compounds as Inhibitor of Dengue Virus (DENV) NS2B/NS3 Protease from Sweet Potato (*Ipomoea batatas* L.) Leaves

Viol Dhea Kharisma[1,2], Rasyadan Taufiq Probojati[1], Ahmad Affan Ali Murtadlo[1], Arif Nur Muhammad Ansori[3], Yulanda Antonius[4], Muhammad Badrut Tamam[1,5]

[1]Researcher, Division of Molecular Biology and Genetics, Generasi Biologi Indonesia Foundation, Gresik, Indonesia, [2]Master Student, Master Program in Biology, Department of Biology, Faculty of Mathematics and Natural Sciences, Brawijaya University, Malang, Indonesia, [3]Doctoral Student, Doctoral Program in Veterinary Science, Faculty of Veterinary Medicine, Universitas Airlangga, Surabaya, Indonesia, [4]Lecturer, Department of Biology, Faculty of Biotechnology, University of Surabaya, Surabaya, Indonesia, [5]Lecturer, Department of Biology, Faculty of Sciences and Technology, Universitas Muhammadiyah Lamongan, Lamongan, Indonesia

Abstract

This study aims to identify the potency of bioactive compounds of sweet potato leaf as inhibitory agent to dengue virus (DENV) NS2B/NS3 protease by using computational study. The 3D structure of NS2B/NS3 protease was collected from PDB and the 2D structure of several bioactive compounds of sweet potato leaf were obtained from PubChem. The visualization and data analysis were performed by using the PyMol software. According to the *in silico* analysis, result demonstrated that dehydroabietinol had the lowest free energy binding. However, based on the protein-ligand analysis, all the compounds showed the hydrogen bond and hydrophobic interaction. All the compounds with hydrogen bond could not be interacted with catalytic domain, but hydrophobic interaction could be interacted to the target domain via Ser135 by δ-Selinene and His51 by α-Caryophyllene. In summary, we conclude that δ-Selinene and α-Caryophyllene might have potencies as a therapeutically drug for dengue.

Keywords: *Dengue virus, in silico, Ipomoea batatas, protease*

Introduction

Indonesia is a tropical country and home of mosquito vector species of dengue virus (DENV), *Aedes aegypti* and *Aedes albopictus*[1]. DENV is infectious agent dengue fever-causing epidemic diseases, current antiviral drug cannot succeed against this entity. Therefore, the development of the drug is required to treat DENV infection[2]. DENV is member family from *Flaviviridae* and consist of four serotypes (DENV 1-4) [3].

Corresponding Authors:
Yulanda Antonius
yulandaantonius@staff.ubaya.ac.id
Muhammad Badrut Tamam
mh.badruttamam@gmail.com

Indonesia is a large country in Southeast Asia and has a high plant diversity in the world. There are more than 5,000 medicinal plants that available all around us[4]. Consequently, medicinal plants used by its population in curing many diseases[5,6]. The medicinal plants generate a variant of chemical composition with the potency to prevent viral replication and probable resource for controlling viral infection[7]. Plants have been described to have antiviral action and some have been accustomed to manage viral taints in humans and animals[8]. Medicinal plants were found for antiviral compounds, such as Convolvulaceae[9].

DENV is a single stranded and positive polarity RNA virus with a genome of about 11,000 bases in length. The genome encodes for three structural proteins and nonstructural proteins, its activated by trypsin-like NS2B/NS3 protease. This enzyme has a catalytic triad domain,

it contains a specific amino acid residual His51, Asp75, and Ser135 required for catalytic activity[10]. Protease complex NS2B/NS3 have a key role in viral replication and make it's as a therapeutic target to development of protease inhibitor for DENV infection[11]. In addition, sweet potato bioactive compounds reported as a potent inhibitor of the virus[12]. Previous research by Pochapski *et al*. (2011) explained that chemical compound contained in sweet potato have potency as a drug but this mechanism action is unknown[13]. Therefore, we identified the potency of bioactive compounds of sweet potato leaf as inhibitory agent to DENV NS2B/NS3 protease by using computational study.

Materials and Methods

Collection of NS2B/NS3 serine protease

The target protein in this research is DENV NS2B/NS3 protease. Therefore, the 3D structure of NS2B/NS3 serine protease was obtained from protein database or RCSB with ID 2FOM. Furthermore, the protein was validated the model quality by using Ramachandran plot.

Collection of sweet potato leaves compounds

Various bioactive compounds from sweet potato leaves referred to previous research[14] were retrieved from PubChem. The 3D structure of compound has collected in structure data format (SDF). Therefore, it must be converted by Open Babel software to produce flexibility 3D structure with protein data bank (PDB) format.

Molecular docking of NS2B/NS3 serine protease with sweet potato leaves compounds

Screening the potency of sweet potato leaves compounds by using virtual screening was conducted with molecular docking. There are several methods which could be applied by using molecular docking, such as specific docking and blind docking[15,16,17]. This research was conducted by using blind docking by PyRx software to identify the potency of bioactive compound from sweet potato leaves as inhibitor NS2B/NS3.

Visualization of interaction between NS2B/NS3 serine protease with sweet potato leaves compounds

Then, we were using PyMol to visualize 3D ligan-protein structure of NS2B/NS3 serine protease and various compounds of sweet potato. Furthermore, those interaction were analyzed by using LigPlot to compared chemical interaction[18,19].

Results and Discussion

DENV is a single stranded and positive polarity RNA virus with a genome of about 11,000 bases in length. The genome encodes for three structural proteins and nonstructural proteins, its activated by trypsin-like NS2B/NS3 protease. This enzyme has a catalytic triad domain, it contains a specific amino acid residual His51, Asp75, and Ser135 required for catalytic activity[10,11]. Protease complex NS2B/NS3 have a key role in viral replication and make it's as a therapeutic target to development of protease inhibitor for DENV infection.

The 3D structure has been obtained from PubChem, around thirty-six of a bioactive compound that's contained in the leaf essential oil of sweet potato, then its minimize by Open Babel because then its minimize by Open Babel because it's will making this ligand have lowest binding energy and generate structure flexibility NS2B/NS3 serine protease (2FOM) obtain from PDB, and then validating structure has been done using RAMPAGE, the result of structure validation showed by Ramachandran plot. Structure validation aims to evaluate the structure quality of targeted protein which is quantify by the number of favored amino acid that reach more than 90%[19]. In this study, targeted protein was visualized based on surfaces structure. Furthermore, the NS2B/NS3 structure is arranged from two chain, A and B which contain α-helix, β-sheet, and coil.

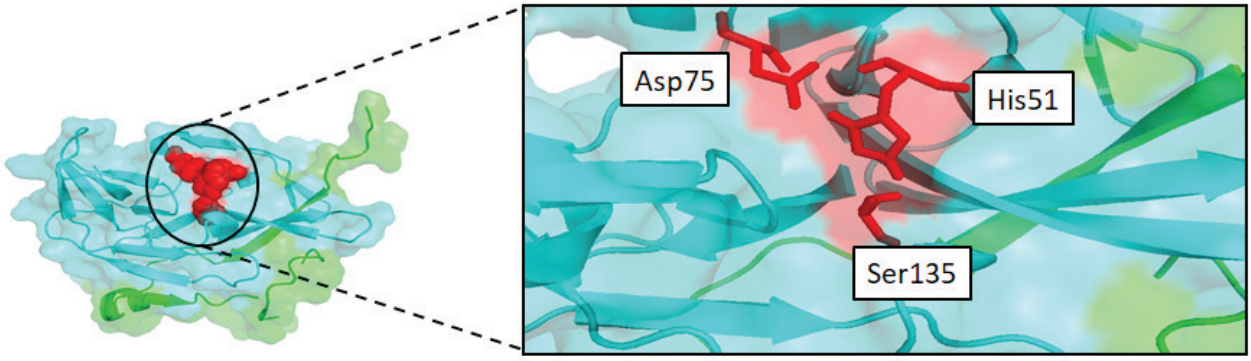

Figure 1. Catalytic triad visualization on NS3/NS2B DENV. Targeted protein was shown in transparent surfaces structure (cyan) and cartoons (green), while the catalytic triad as drug target shown in stick structure colored in red to distinguish the drug target domain with the others.

Molecular docking is a part of in silico analysis that has main objective to identify the energy binding size and the interaction pattern between protein and its ligand according to the chemical interaction within the complex[16]. Molecular docking has performed by PyRx software to know binding affinity level with grid positions x: -0,4637 y: -15,1662 z: 16,1087 and dimensions (Å) x: 52,1952 y: 56,6277 z: 46,8960 reffer to catalytic site domain on NS2B/NS3 serine protease with amino acid residual is His51, Asp75, and Ser135, that be visualized by PyMol software as stick in cartoon structure with surface on target protein (Figure 1). After we know the positions of the catalytic site, then docking grid was directed to its. Docking result indicated that compound has a lowest binding affinity is dehydroabietinol around -7,1 kcal/mol. We revealed another results, such as abietadiene (-6.9 kcal/mol), cembrene (-6.6 kcal/mol), δ-selinene (-6.5 kcal/mol), δ-cadinene (-6.4 kcal/mol), spathulenol (-6.2 kcal/mol), β-cuvebene (-6.0 kcal/mol), γ-gurjunene (-5.9 kcal/mol), α-bergamotenol (-5.8 kcal/mol), β-caryophyllene (-5.8 kcal/mol), β-elemene (-5.8 kcal/mol), allo-aromadendrene (-5.7 kcal/mol), β-chamigrene (-5.7 kcal/mol), β-panasinsene (-5.7 kcal/mol), trans-α-bergamotene (-5.7 kcal/mol), caryophyllene oxide (-5.6 kcal/mol), γ-elemene (-5.6 kcal/mol), longifolene (-5.6 kcal/mol), α-caryophyllene (-5.5 kcal/mol), α-thujene (-5.5 kcal/mol), octadecanoic acid (-5.5 kcal/mol), bicyclogermacrene (-5.4 kcal/mol), limonene (-5.3 kcal/mol), terpinen-4-ol (-5.3 kcal/mol), eugenol (-5.2 kcal/mol), n-hexadecanoic acid (-5.2 kcal/mol), α-farnesene (-5.1 kcal/mol), α-santalol (-5.1 kcal/mol), γ-terpinene (-5.1 kcal/mol), p-cymene (-5.1 kcal/mol), p-menth-1-ene (-5.1 kcal/mol), bicycloelemene (-5.0 kcal/mol), α-pinene (-4.8 kcal/mol), β-pinene (-4.8 kcal/mol), cis-sabinene (-4.8 kcal/mol), and 1-octen-3-Ol (-4.5 kcal/mol). Binding affinity is energy bonding formed from the interactions some molecule with other, several parameters affect binding affinity such as amino acid residues and type of chemical interaction between ligand-protein such hydrogen, hydrophobic, and Van der Waals. Binding affinity commonly used as indicator of binding energy to determine the complex interaction which is considering as biological activity outcome[16].

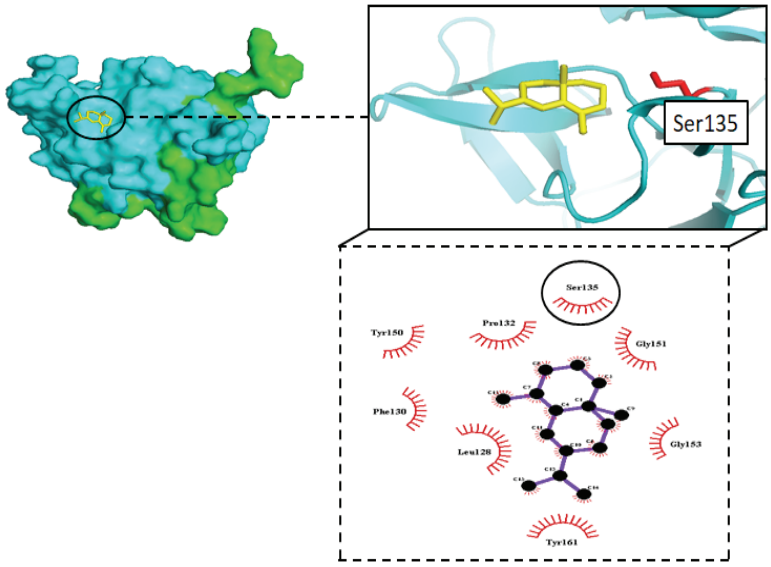

Figure 2. Targeted domain and δ-Selinene interaction. The ligand was shown as yellow stick structure, while the specific residual amino acid was shown as red color. The hydrophobic interaction was occurring in Ser135 area shown in black circle.

Based on results of molecular docking, a bioactive compound from sweet potato leaves have a potency to bind NS2B/NS3 with lowest binding affinity and possible formed stable complex of ligand-protein. The amount of free energy (ΔG) indicating as an ability of binding for a bioactive compound to the target protein. In this condition, the ligand bind to target protein and making of energy alteration such Gibbs free energy (ΔG), it has negative value when the system in equilibrium condition with constant pressure and temperature, because the widely of protein-ligand association can be determined by negative ΔG, so its determination of the protein-ligand complex or ligand binding affinity[20].

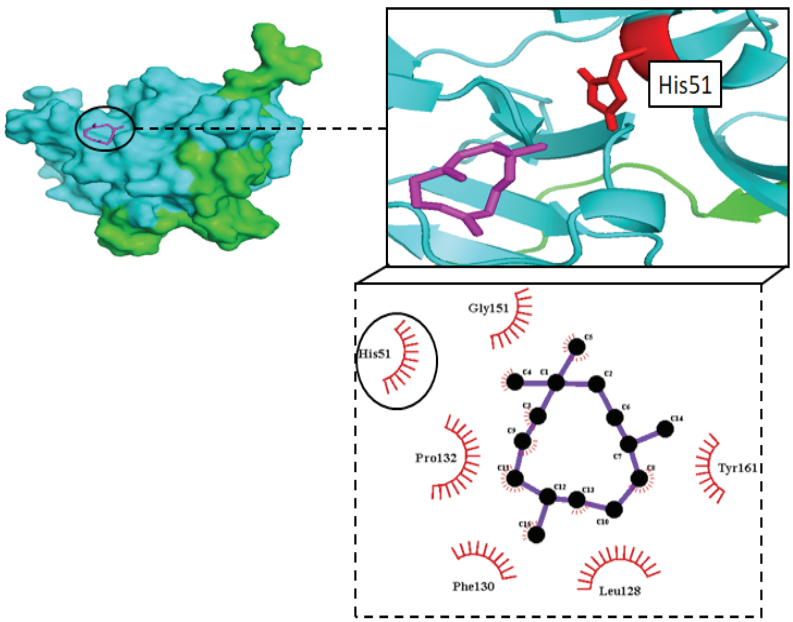

Figure 3. The α-Caryophyllene interaction to targeted domain. The ligand was shown as purple stick structure, while the red color is the residual amino acid in NS2B/NS3. The hydrophobic interaction was occurring in Ser135 which shown inside the black circle.

Potency as inhibitor NS2/NS3 serine protease in the oil essential of sweet potato leaves showing dehydroabietinol have lowest free energy binding, but refer to the result of analysis of protein-ligand domain interaction of the all compound showing, it's had two type of chemical interaction between ligand with protein domain as hydrogen bond and hydrophobic. All of the compounds have hydrogen bond cannot be interacted with catalytic domain, but hydrophobic interaction can be interacted to target domain, via Ser135 by δ-Selinene (Figure 2) and His51 by α-Caryophyllene (Figure 3). Catalytic triad (Ser135, His51, and Asp75) can be found in NS2B/NS3 and required to protease activity which functions as a mechanism for activation of DENV replication[11]. So, it is predicted that the two compounds are very possible to interact with the catalytic site domain in NS2B/NS3. Therefore, it can be potentially as an inhibitor compare to dehydroabietinol which has lower binding affinity without chemical interaction site in targeted domain in NS2/NS3 serine protease.

Conclusion

In summary, the δ-Selinene and α-Caryophyllene are predicted to have potency as dengue disease medication through the inhibitory mechanism against DENV. Specifically, the ligands are binding to one of catalytic triad of residual amino acid. This interaction inhibits the targeted protein activation when the virus replication occurs.

Conflict of Interest: The author declare that they have no conflict of interest.

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Ethical Approval: No ethical approval needed.

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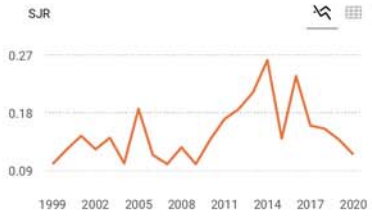

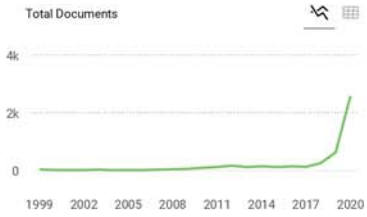

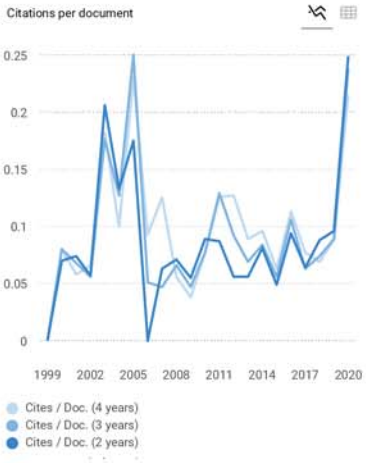

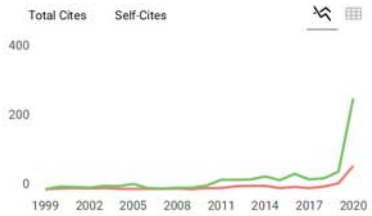

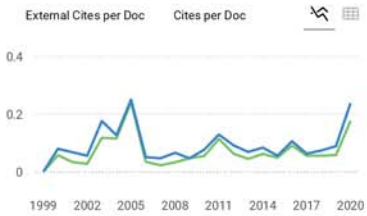

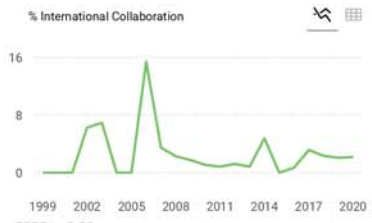

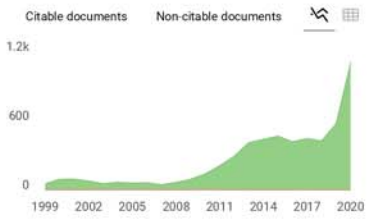

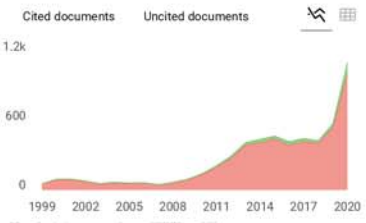

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Hello, I am the researcher Aqeel.
A research has been published in your journal entitled
(Treatment and experimental infection with Klebsiella
pneumoniae in Rats)
It has not yet appeared on the Scopus page. Please reply to this message to find out the reason

reply

SCImago Team

Melanie Ortiz 2 years ago

Dear Aqueel,
thank you very much for your comment, unfortunately we cannot help you with your request. We suggest you to contact directly with Scopus support:
https://service.elsevier.com/app/answers/detail/a_id/14883/kw/scimago/supporthub/scopus/
Best Regards, SCImago Team

D **Dr. Fouad Fadhil Al-Qaim** 2 years ago

Dear Sir/Madam
I have only one question.
How does the same journal gather between science and social science (toxicology and law)?
Please can you explain, why it was considered in SJR data base?
Thank you

reply

SCImago Team

Melanie Ortiz 2 years ago

Dear Fouad,
Thank you for contacting us.
SJR is a portal with scientometric indicators of journals indexed in Scopus. All the data (Category, Publisher, etc) have been provided By Scopus /Elsevier and SCImago doesn´t have the authority over this data which are property of Scopus/Elsevier. SCImago has a signed agreement that limits our performance to the generation of scientometric indicators derived from the metadata sent in the last update.
We suggest you to contact with Scopus support regarding this matter:
https://service.elsevier.com/app/answers/detail/a_id/14883/kw/scimago/supporthub/scopus/

Best Regards, SCImago Team

A **aarti** 2 years ago

sir I want to publish my article and I have prepared accordinly but not able to find the copyright form. please help

reply

B **Bahram** 2 years ago

Hello my dear

Please answer my questions

1 - On what bases does your magazine index? (ISI. Pub med or Scopus)?

2 - How many weeks is the maximum arbitration time? Is it possible to make quick judgments?

3 - How much does it cost to print an article?

Thank you

reply

H **hanaa** 2 years ago

Hello dear: When will the 14th volume of the Indian Journal of Forensic Medicine and Toxicology be published?

SCImago Team

Melanie Ortiz 2 years ago

Dear Hanaa,
thank you for contacting us.
Unfortunately, we cannot help you with your request, we suggest you to visit the journal's homepage or contact the journal's editorial staff , so they could inform you more deeply.
Best Regards, SCImago Team

SCImago Team

Melanie Ortiz 2 years ago

Dear Bahram,,
thank you for contacting us.
We are sorry to tell you that SCImago Journal & Country Rank is not a journal. SJR is a portal with scientometric indicators of journals indexed in Elsevier/Scopus. We suggest you to consult Scopus and/or other databases to know where is this journal indexed in. You can also check that information in the journal's website or contact directly with the editorial staff. For further information about this journal, please visit the journal's website.Best Regards, SCImago Team

A **AUTHOR** 2 years ago

is this journal still under scopus..??

reply

T **Tri Astuti Sugiyatmi** 7 months ago

After May 2021, is this journal still indexed by Scopus?

Warm Regard

Tri

SCImago Team

Melanie Ortiz 7 months ago

Dear Tri Astuti,
Thank you very much for your comment.
All the metadata have been provided by Scopus /Elsevier in their last update sent to SCImago, including the Coverage's period data. The SJR for 2020 has been released on 17 May 2021. We suggest you consult the Scopus database directly to see the current index status as SJR is a static image of Scopus, which is changing every day.
Best Regards, SCImago Team

R **Raian Zobi** 7 months ago

Is journal still under scopous?

SCImago Team

Melanie Ortiz 7 months ago

Dear Raian,
Thank you very much for your comment.
All the metadata have been provided by Scopus /Elsevier in their last update sent to SCImago, including the Coverage's period data. The SJR for 2020 has been released on 17 May 2021. We suggest you consult the Scopus database directly to see the current index status as SJR is a static image of Scopus, which is changing every day.
Best Regards, SCImago Team

SCImago Team

Melanie Ortiz 2 years ago

Dear Sir/Madam, thank you very much for your comment, unfortunately we cannot help you with your request. We suggest you to consult the Scopus database directly. Keep in mind that the SJR is a static image (the update is made one time per year) of a database (Scopus) which is changing every day.
Best Regards, SCImago Team

D **Dr. Shalender Kumar, MD (FM)** 3 years ago

Sir, I want to submit my manuscript for publication in your journal. So sir on which mail id I can do it sir. Kindly guide me sir. Thanks and regards.

reply

SCImago Team

Elena Corera 3 years ago

Dear Dr Shalender,

thank you very much for your comment, unfortunately we cannot help you with your request. We suggest you check author's instructions in journal website. You can find that information in SJR website https://www.scimagojr.com

Best Regards,
SCImago Team

Leave a comment

Name

Email
(will not be published)

Submit

The users of Scimago Journal & Country Rank have the possibility to dialogue through comments linked to a specific journal. The purpose is to have a forum in which general doubts about the processes of publication in the journal, experiences and other issues derived from the publication of papers are resolved. For topics on particular articles, maintain the dialogue through the usual channels with your editor.

Developed by: SCImago

Powered by: Scopus

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Source details

Indian Journal of Forensic Medicine and Toxicology

Scopus coverage years: from 2008 to 2021
(coverage discontinued in Scopus)
Publisher: Institute of Medico-Legal Publications
ISSN: 0973-9122 E-ISSN: 0973-9130
Subject area: Social Sciences: Law | Medicine: Pathology and Forensic Medicine | Pharmacology, Toxicology and Pharmaceutics: Toxicology | Environmental Science: Health, Toxicology and Mutagenesis
Source type: Journal

CiteScore 2020
0.1

SJR 2020
0.115

SNIP 2020
0.243

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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

$$0.1 = \frac{387 \text{ Citations } 2017 - 2020}{3{,}509 \text{ Documents } 2017 - 2020}$$

Calculated on 05 May, 2021

CiteScore rank 2020

Category	Rank	Percentile
Social Sciences Law	#639/722	11th
Medicine Pathology and Forensic Medicine	#183/191	4th
Pharmacology, Toxicology and	#118/122	3rd

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Indian Journal of Forensic Medicine & Toxicology

Editorial Team

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Articles