Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

Bukti Korespondensi

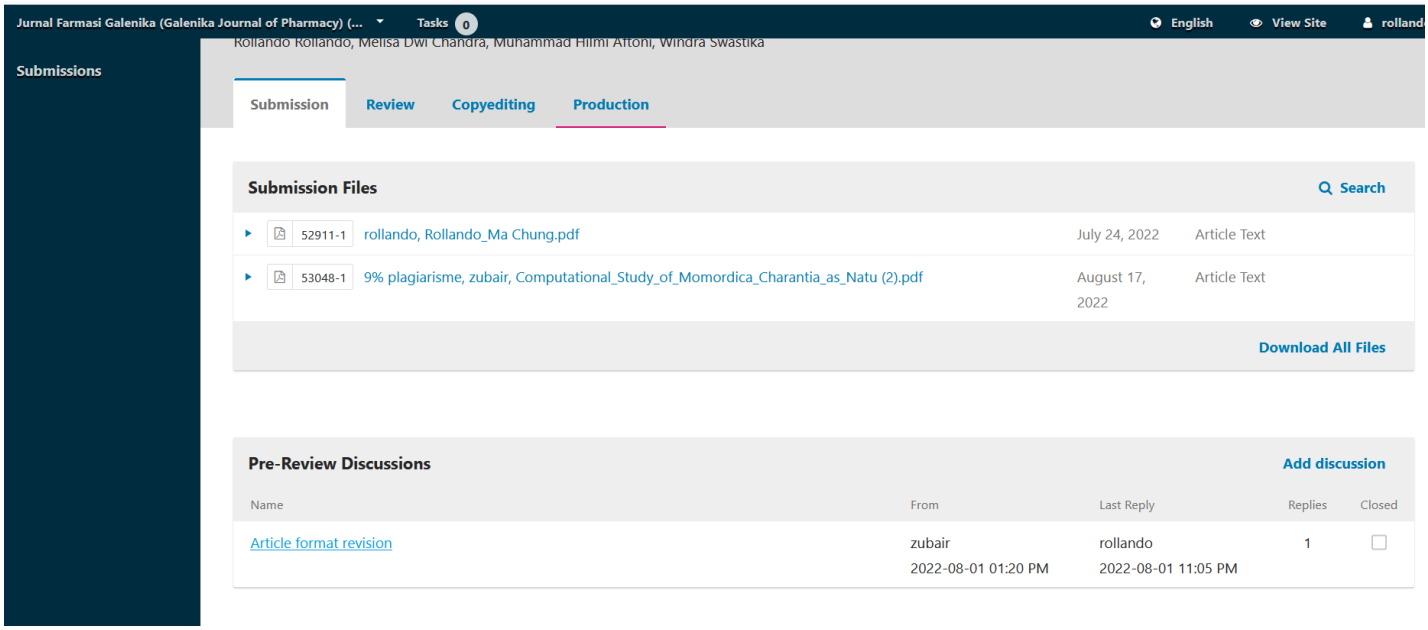
Judul Artikel: Molecular Docking and Molecular Dynamic Studies of Secondary Metabolites from Momordica Charantia as Natural Antidiabetic

No	Proses	Tanggal
1	Author mengirimkan artikel ke Jurnal Galenika	24-7-2022
2	Editor mengirimkan hasil review pertama	27-9-2022
3	Author mengirimkan hasil perbaikan artikel yang pertama	3-10-2022
4	Editor mengirimkan hasil review kedua	18-2-2023
5	Author mengirimkan hasil perbaikan artikel yang kedua	4-3-2023
6	Editor menyampaikan bahwa artikel diterima untuk diterbitkan	5-6-2023
7	Editor menyampaikan bahwa artikel masuk pada proses editing lay out	11-3-2024
8	Artikel dipublikasi pada Jurnal Farmasi Galenika Vol. 10, No.1 (2024).	11-3-2024

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

1. Author mengirimkan artikel ke Jurnal Galenika (24-7-2022)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala



Article format revision

Participants

Muhammad Sulaiman Zubair, Ph.D (zubair)

rollando rollando (rollando)

Messages

Note	From
Please submit manuscript on microsoft word format (.docx)	zubair 2022-08-01 01:20 PM
Terimakasih atas saran yang diberikan. Saya mengirim dalam bentuk pdf karena file kami terlalu besar. Akibatnya, tidak dapat di submit secara langsung ke OJS. Saya akan kirimkan file dalam bentuk word. Terimakasih rollando, Artikel_Revisi.docx	rollando 2022-08-01 11:05 PM

Add Message

2. Editor mengirimkan hasil review pertama (27-9-2022)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

Notifications

[JFG] Editor Decision

2022-09-27 03:06 AM

rollando rollando:

We have reached a decision regarding your submission to Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal), "Computational Study of Momordica Charantia as Natural Antidiabetic".

Our decision is: Revisions Required

Please note that you have to submit the revised version of your manuscript as soon as possible with the respond to reviewers comments by answering their comments point by point in a separated file (rebuttal letter).

We will not process the manuscript if the manuscript was not revised as reviewer suggestion or if there is no a rebuttal letter

Thanks and regards

Muhammad Sulaiman Zubair, Ph.D
Tadulako University
sulaiman_zubair80@yahoo.co.id

Reviewer A:
Recommendation: Revisions Required

Reviewer Comment

Please attach proof reading in this manuscript

Prof. Apt. M. Sulaiman Zubair, PhD

Editor in Chief

Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)

Antidiabetic Activity Test on Momordica Charantia In Silico

Commented [LI1]: Computational Study of Momordica Charantia as Natural Antidiabetic or Antidiabetic Activity Test on Momordica Charantia In Silico ?

ABSTRACT

Background: Diabetes Mellitus is a non-communicable disease characterized by hyperglycemia. Diabetes mellitus occurs when the body cannot receive or use insulin properly. If you already have diabetes, then the patient must take medication continuously because diabetes mellitus is a lifelong disease. Because medicines are quite expensive, alternative ways to cure the disease are needed by consuming traditional medicines, one of which is bitter melon (Momordica charantia). **Objectives:** This study is aimed to find out the compound metabolites, molecular interactions and knowing what compounds found in bitter melon plants which have the potential to lower blood sugar. **Material and Methods:** 12 compounds from the Momordica charantia planta nd 6 proteins (1IR3, 1RHF, 1XU7, 4PNZ, 4YVP, 2NT7) that will be docked using Pymol, Pyrx, Biovia Discovery Studio and YASARA applications. **Results:** ~~From the results of the docking that has been carried out,~~ three compounds have the highest binding affinity values, namely momordenol, oleanolic acid ~~compound~~, and momordicin I. Next, the YASARA test was carried out. In this test, it was found that RMSD<2Å. RMSD<2Å can indicate that the research conducted is valid and the method used is correct. **Conclusions:** Momordica charantia plant has potential activity as antidiabetic.

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Commented [LI5]: Refer to the specific docking tools only

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Keywords: In Silico, Momordica charantia, molucular docking, molecular dynamic

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Commented [LI9]: As antidiabetic based on in silico study

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ABSTRAK

Latar Belakang: Diabetes Mellitus merupakan penyakit tidak menular yang ditandai dengan terjadinya hiperglikemia. Diabetes mellitus terjadi ketika tubuh tidak dapat menerima atau menggunakan insulin dengan baik. Jika sudah mengidap diabetes, maka penderita harus minum obat terus menerus karena diabetes melitus merupakan penyakit seumur hidup. Karena obat-obatan cukup mahal, maka diperlukan cara alternatif untuk menyembuhkan penyakit tersebut dengan mengkonsumsi obat-obatan tradisional, salah satunya pare (Momordica charantia). **Tujuan Penelitian:** bertujuan untuk mengetahui senyawa metabolit, interaksi molekuler dan mengetahui senyawa apa saja yang terdapat pada tanaman pare yang berpotensi menurunkan gula darah. **Bahan dan Metode:** 12 senyawa dari Momordica charantia planta nd 6 protein (1IR3, 1RHF, 1XU7, 4PNZ, 4YVP, 2NT7) yang akan di-docking menggunakan aplikasi Pymol, Pyrx, Biovia Discovery Studio dan YASARA. **Hasil:** Dari hasil docking yang telah dilakukan, terdapat tiga senyawa yang memiliki nilai afinitas ikatan tertinggi yaitu momordenol, senyawa asam oleanolat, dan momordisin I. Selanjutnya dilakukan uji YASARA. Pada pengujian ini didapatkan bahwa RMSD<2Å. RMSD<2Å dapat menunjukkan bahwa penelitian yang dilakukan adalah valid dan metode yang digunakan sudah benar. **Kesimpulan:** Tanaman *Momordica charantia* memiliki potensi aktivitas sebagai antidiabetik.

Kata kunci: In Silico, Momordica charantia, molekuler dinamik, molukuler docking

INTRODUCTION

Diabetes mellitus (DM) is a non-communicable disease that arises due to metabolic disorders in the body that cause the body's inability to use blood glucose which causes glucose to accumulate in the blood. Diabetes mellitus is characterized by hyperglycemia and disorders of carbohydrate, protein and fat metabolism associated with insulin secretion abnormalities or lack of insulin secretory action. The signs experienced by people with diabetes mellitus are frequent thirst, frequent urge to urinate, polyphagia, drastic weight loss, and tingling. Diabetes mellitus is divided into 4, namely: type 1, type 2 diabetes mellitus, diabetes mellitus due to other causes, and gestational diabetes (Association, 2018).

In the treatment of diabetes usually many people use antidiabetic drugs. In addition to relatively long treatment and the price is quite expensive, diabetes drugs usually cause unwanted side effects. Therefore, the use of traditional medicine is the best solution for the treatment of diabetes mellitus. Traditional medicine is a non-drug therapy that is proven to be safer and does not cause many

MATERIAL AND METHODS

Materials

The design used for this research is the experimental method. ~~This research was conducted at home independently.~~ The material used is protein from antidiabetic along with compounds found in bitter melon plants (momordica charantia). ~~The tools used are hardware and software.~~ ~~Hardware in the form of~~ a laptop with ram specifications ~~(random access memory)~~ 4 gigabyte, processor intel (r) celeron CPU N3350 1.10ghz (2 cpus). The software used is windows 10 (home Single language 64 bit), Pubchem program, Open Babel ~~application~~, ~~program~~ String, Pyrx ~~app~~, PyMOL ~~app~~, Discovery Studio 2021, PDB ~~program~~ (Data Bank Protein), PDBsum program and PASS Online, YASARA application.

Methods

Search For Bitter Melon Plant Activity

A search for bitter melon (Momordica charantia) compounds was conducted on the knapsackfamily.com website. After getting the bitter melon compound, then the compound is downloaded on the website https://pubchem.ncbi.nlm.nih.gov/. On this website, download the compound along with the SMILES (Simplified Molecular Input Life Entry System) copy of the compound for further testing. The downloaded compound structure must be in 3D with sdf format. If the 3D Sdf structure cannot be found on the website, it can be downloaded in the form of 2D Sdf which must be downloaded first and converted to 3D Sdf using the Open Babel application.

Activity Test and Characteristic Test of Bitter Melon

The copied SMILES are then tested for PASS on the https://way2drug.com/ website. After that, the activity display of the compound will appear. Then select a compound that has Pa>0.7. The next step is to perform the ADMET test. The ADMET test is carried out by entering SMILES on the pkCSM ~~website at~~ https://www.biosig.unimelb.edu.au. The pkCSM website is needed to identify compounds that act as drugs.

2

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Diabetic Protein Search for Molecular Docking

In the docking molecule, the protein is downloaded via the PDB database ~~program on the website~~ (https://www.rcsb.org). In choosing protein in PDB, try to meet the requirements, namely for the resolution limit of 1-3. In this case the smaller it is, the better it will be and missing residue is avoided (dotted line contained in the protein) in addition, in the selection of the protein must first be checked by the Ramachandran plot in the protein.To view the Ramachandran plot, please visit the website www.ebi.ac.uk. In the website Ramachandran was chosen more than 90% because the protein has completed amino acids. After download the protein is searched for native ligands using an application PyMOL.

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Protein Preparation and Visualization

The protein preparation required the application of PyMOL. this app to remove water molecules. Water molecules must be removed beforehand so as not to interfere during the docking process and to ensure that what is done for docking is really the original compound and receptor.

Commented [LI32]: Please include citations in this statement, only for water molecules? How about the others solvent residue?

Docking Process

Docking process using the Pyrx application. The first step in molecular docking is to enter the prepared protein then right click select autodock and select make to macromolecule. To enter native ligands and compounds to be used, this can be done by clicking open babel contained in the application and then entering the desired compound, right click select minimize all energy then right click again select convert all to autodock ligand pdbqt. then enter the vina wizard and start here then enter the protein and the desired ligand and select forward. The results of Pyrx with the output of pdbqt can be seen from the interaction via the following table which has appeared after docking. Then select the smallest ΔG value for each available interaction.

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2. Please provide grid box volume and coordinates that have been used in this research

Visualization of The Bond Between Protein and Ligand

Open the Discovery Studio 2021 application, then open the docking file in the complex folder then select receptor-ligand interaction then ligand interaction and then display a 2D diagram. Then the interaction between the ligand and protein will appear. After the ligand and receptor binding results are obtained, the next step is to enter the YASARA application. YASARA program is used to see RMSD (Root Mean Square Deviation). RMSD is a parameter commonly used to evaluate the similarity of two structures based on differences in similar atomic distances. The way to measure RMSD with YASARA is to open the original ligand file then overlay it with the best conformation file of tethering. Then by running the "Analyze > RMSD of" function on YASARA, the RMSD value of protein binding with the original ligand can be obtained. Proteins with an RMSD value of more than 2.00Å are considered invalid and cannot be used for tethering with other ligands, because the bond distance will not be optimal. , a protein with an RMSD of less than 2.00Å which will be used as a test protein to perform a molecular docking test

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RESULTS AND DISCUSSION

Bitter Melon Plant Compounds

After a search, several compounds of bitter melon were found. In this research, 12 compounds were used. The 12 compounds can be seen in table 1.

Table 1. Compounds of Bitter Melon

No	Compound	Group	Source
1.	*9t,11t,13t conjugated linoleic acid*	*Tyrterpenoid*	(Hsu et al., 2011)
2.	*Arginine*	Fenolik	(Y. Ulung Anggraito, R. Susanti, 2018)
3.	*Benzoic acid*	*Flavonoid*	(Jia et al., 2017)
4.	*Conjugated linoleic acid*	*Tryterpenoid*	(Hsu et al., 2011)
5.	*Linoleic acid*	*Tryterpenoid*	(Hsu et al., 2011)
6.	*Momordenol*	*Tryterpenoid*	(Torre et al., 2020)
7.	*Momordicin I*	*Tryterpenoid*	(Torre et al., 2020)
8.	*Niacin*	Vitamin	(Rizeki et al., 2012)
9.	*Oleanolic acid*	*Flavonoid*	(Jia et al., 2017)
10.	*Pectin*	Polisakarida	(Nur Wana, 2013)
P11.	*Phenylalanine*	Fenolik	(Y. Ulung Anggraito, R. Susanti, 2018)
12.	*Phenol*	Fenolik	(Torre et al., 2020)

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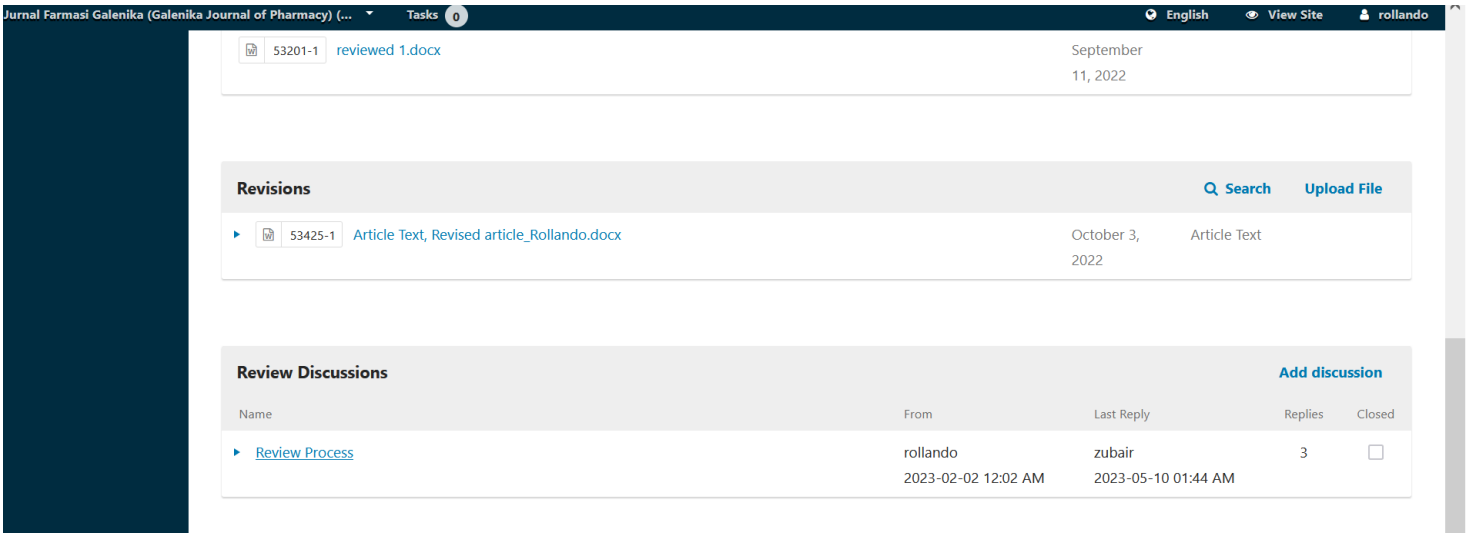
After obtaining the compound that will be used, the SMILES search for the compound is then carried out. SMILES of 12 compounds can be seen in table 2.

Table 2. SMILES of Bitter Melon

No	Compound	SMILES
1.	*9t,11t,13t conjugated linoleic acid*	OC(CCCCCCC/C=C/C=C/C=C/CCCC)=O
2.	*Arginine*	OC([C@H](CCCN=C(N)N)N)=O
3.	*Benzoic acid*	OC(C1=CC=CC=C1)=O
4.	*Conjugated linoleic acid*	OC(CCCCCCC/C=C/C=C/C=C/CCCC)=O
5.	*Linoleic acid*	OC(CCCCCCC/C=C\C/C=C\CCCCC)=O
6.	*Momordenol*	O=C1[C@H]([C@H](C)CC[C@H](CC)C(C)C)[C@@]2(C)C([C@@H]3[C@@H](CC2)[C@@](CC[C@H]4O)(C)C(C4)=CC3)=C1
7.	*Momordicin I*	O[C@@H]1[C@H]([C@@]([C@H](CC[C@@H]2O)C(C2(C)C)=C1)(C=O)CC3)[C@@]4(C)[C@@]3(C)[C@@H]([C@H](C)C[C@@H](C=C(C)C)O)CC4
8.	*Niacin*	OC(C1=CN=CC=C1)=O

3. Author mengirimkan hasil perbaikan artikel yang pertama (3-10-2022)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala



Computational Study of Momordica Charantia as Natural Antidiabetic

ABSTRACT

Background: Diabetes Mellitus is a non-contagious disease characterized by hyperglycemia. Diabetes mellitus occurs when the body cannot receive or use insulin properly. If you already have diabetes, then the patient must take medication continuously because diabetes mellitus is a lifelong disease. Because medicines are quite expensive, alternative ways to cure the disease are needed by consuming traditional medicines, one of which is bitter melon (Momordica charantia). **Objectives:** This study is aimed to find out the compound metabolites, molecular interactions and reveal potential compoundsin bitter melon plants which have the potential to lower blood sugar. **Material and Methods:** 12 compounds from the *Momordica charantia* planta nd 6 proteins (1IR3, 1RHF, 1XU7, 4PNZ, 4YVP, 2NT7) that will be docked using Pyrx and YASARA applications. **Results:** Three compounds have the highest binding affinity values, namely momordenol, oleanolic acid, and momordicin. The results of the molecular dynamics test showed that the three compounds were stable in interacting with the proteins 1IR3, 1RHF, 4PNZ, 4YVP, 1XU7, and 2NT7. ADMET test showed that momordenol, oleanolic acid, and momordicin had drug-like characteristics. The docking protocol was carried out with ligand and protein preparation, then continued with internal validation with native ligands. it was found that RMSD<2Å. RMSD<2Å can indicate that the research conducted is valid and the method used is correct. **Conclusions:** Momordica charantia plant has potential activity as antidiabetic based on in silico study.

Keywords: In Silico, *Momordica charantia*, molucular docking, molecular dynamic

ABSTRAK

Latar Belakang: Diabetes Mellitus merupakan penyakit tidak menular yang ditandai dengan terjadinya hiperglikemia. Diabetes mellitus terjadi ketika tubuh tidak dapat menerima atau menggunakan insulin dengan baik. Jika sudah mengidap diabetes, maka penderita harus minum obat terus menerus karena diabetes melitus merupakan penyakit seumur hidup. Karena obat-obatan cukup mahal, maka diperlukan cara alternatif untuk menyembuhkan penyakit tersebut dengan mengkonsumsi obat-obatan tradisional, salah satunya pare (Momordica charantia). **Tujuan Penelitian:** bertujuan untuk mengetahui senyawa metabolit, interaksi molekuler dan mengetahui senyawa apa saja yang terdapat pada tanaman pare yang berpotensi menurunkan gula darah. **Bahan dan Metode:** 12 senyawa dari Momordica charantia planta nd 6 protein (1IR3, 1RHF, 1XU7, 4PNZ, 4YVP, 2NT7) yang akan di-docking menggunakan aplikasi Pyrx dan YASARA. **Hasil:** Dari hasil docking yang telah dilakukan, terdapat tiga senyawa yang memiliki nilai afinitas ikatan tertinggi yaitu momordenol, senyawa asam oleanolat, dan momordisin. Hasil uji dinamika molekuler menunjukkan ketiga senyawa tersebut stabil berinteraksi dengan protein 1IR3, 1RHF, 4PNZ, 4YVP, 1XU7, dan 2NT7. Uji ADMET menunjukkan bahwa senyawa momordenol, oleanolic acid, dan momordisin memiliki karakter mirip obat. Protokol docking dilakukan dengan preparasi ligan dan protein, kemudian dilanjutkan dengan validasi internal dengan ligand asli. Pada pengujian ini didapatkan bahwa RMSD<2Å. RMSD<2Å dapat menunjukkan bahwa penelitian yang dilakukan adalah valid dan metode yang digunakan sudah benar. **Kesimpulan:** Tanaman *Momordica charantia* memiliki potensi aktivitas sebagai antidiabetik.

Kata kunci: In Silico, Momordica charantia, molekuler dinamik, molukuler docking

INTRODUCTION

Diabetes mellitus (DM) is a non-communicable disease that arises due to metabolic disorders in the body that cause the body's inability to use blood glucose which causes glucose to accumulate in the blood. Diabetes mellitus is characterized by hyperglycemia and disorders of carbohydrate, protein and fat metabolism associated with insulin secretion abnormalities or lack of insulin secretory action. The signs experienced by people with diabetes mellitus are frequent thirst, frequent urge to urinate, polyphagia, drastic weight loss, and tingling. Diabetes mellitus is divided into 4, namely: type 1, type 2 diabetes mellitus, diabetes mellitus due to other causes, and gestational diabetes (Association, 2018).

MATERIAL AND METHODS

Materials

The design used for this research is the experimental method. The material used is protein from antidiabetic (1IR3, 1RHF, 4PNZ, 4YVP, 1XU7, and 2NT7) along with compounds found in bitter melon plants (*Momordica charantia*) (http://www.knapsackfamily.com). The hardware is a laptop with ram specifications 4 gigabyte, processor intel (r) celeron CPU N3350 1.10ghz (2 cpus). The OS used is windows 10 (64 bit), Pubchem database, Open Babel, String, Pyrx, PyMOL, Discovery Studio 2021, PDB (https://www.rcsb.org/), PDBsum program (https://www.ebi.ac.uk) and PASS Online (https://www.passonline.org), and YASARA.

Methods

Search For Bitter Melon Plant Activity

A search for bitter melon (*Momordica charantia*) compounds were conducted on the KNApSAcK family website. After getting the bitter melon compound, then the compound is downloaded on the website https://pubchem.ncbi.nlm.nih.gov/. On this website, download the compound along with the SMILES (Simplified Molecular Input Life Entry System) copy of the compound for further testing. The downloaded compound structure must be in 3D with .sdf format. If the 3D Sdf structure cannot be found on the website, it can be downloaded in the form of 2D sdf which must be downloaded first and converted to 3D sdf using the Open Babel application.

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Protein Preparation and Visualization

The protein preparation required the application of PyMOL. this app to remove water molecules. Water molecules and solvent residue must be removed beforehand so as not to interfere during the docking process and to ensure that what is done for docking is really the original compound and receptor (Karyawati, 2020).

Docking Process

Docking process using the Pyrx application. The first step in molecular docking is to enter the prepared protein then right-click select autodock and select make to the macromolecule. To enter native ligands and compounds to be used, this can be done by clicking open babel contained in the application and then entering the desired compound, right click select minimize all energy than right click again select convert all to autodock ligand pdbqt. then enter the vina wizard and start here then enter the protein and the desired ligand and select forward. The results of Pyrx with the output of pdbqt can be seen from the interaction via the following table which appeared after docking. Then select the smallest DG value for each available interaction

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RESULTS AND DISCUSSION

Bitter Melon Plant Compounds

After a search, several compounds of bitter melon were found. In this research, 12 compounds were used. The 12 compounds can be seen in table 1.

Table 1. Compounds of Bitter Melon

No	Compound	Group	Source
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2.	*Arginine*	*Phenolic*	(Y. Ulung Anggraito, R. Susanti, 2018)
3.	*Benzoic acid*	*Flavonoid*	(Jia et al., 2017)
4.	*Conjugated linoleic acid*	*Tryterpenoid*	(Hsu et al., 2011)
5.	*Linoleic acid*	*Tryterpenoid*	(Hsu et al., 2011)
6.	*Momordenol*	*Tryterpenoid*	(Torre et al., 2020)
7.	*Momordicin I*	*Tryterpenoid*	(Torre et al., 2020)
8.	*Niacin*	Vitamin	(Rizeki et al., 2012)
9.	*Oleanolic acid*	*Flavonoid*	(Jia et al., 2017)
10.	*Pectin*	*Polysaccharide*	(Nur Wana, 2013)
P11.	*Phenylalanine*	*Phenolic*	(Y. Ulung Anggraito, R. Susanti, 2018)
12.	*Phenol*	*Phenolic*	(Torre et al., 2020)

After obtaining the compound that will be used, the SMILES search for the compound is then carried out. SMILES of 12 compounds can be seen in table 2.

Table 2. SMILES of Bitter Melon

No	Compound	SMILES
1.	*9t,11t,13t conjugated linoleic acid*	OC(CCCCCCC/C=C/C=C/C=C/CCCC)=O
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3.	*Benzoic acid*	OC(C1=CC=CC=C1)=O
4.	*Conjugated linoleic acid*	OC(CCCCCCC/C=C/C=C/C=C/CCCC)=O
5.	*Linoleic acid*	OC(CCCCCCC/C=C\C/C=C\CCCCC)=O
6.	*Momordenol*	O=C1[C@H]([C@H](C)CC[C@H](CC)C(C)C)[C@@]2(C)C([C@@H]3[C@@H](CC2)[C@@](CC[C@H]4O)(C)C(C4)=CC3)=C1
7.	*Momordicin I*	O[C@@H]1[C@H]([C@@]([C@H](CC[C@@H]2O)C(C2(C)C)=C1)(C=O)CC3)[C@@]4(C)[C@@]3(C)[C@@H]([C@H](C)C[C@@H](C=C(C)C)O)CC4
8.	*Niacin*	OC(C1=CN=CC=C1)=O

4. Editor mengirimkan hasil review kedua (18-2-2023)

Notifications

[JFG] Editor Decision

2023-02-18 12:44 AM

rollando rollando:

We have reached a decision regarding your submission to Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal), "Computational Study of Momordica Charantia as Natural Antidiabetic".

Our decision is: Revisions Required

Please note that you have to submit the revised version of your manuscript as soon as possible with the respond to reviewers comments by answering their comments point by point in a separated file (rebuttal letter).

We will not process the manuscript if the manuscript was not revised as reviewer suggestion or if there is no a rebuttal letter

Thanks and regards

Muhammad Sulaiman Zubair, Ph.D
Tadulako University
sulaiman_zubair80@yahoo.co.id

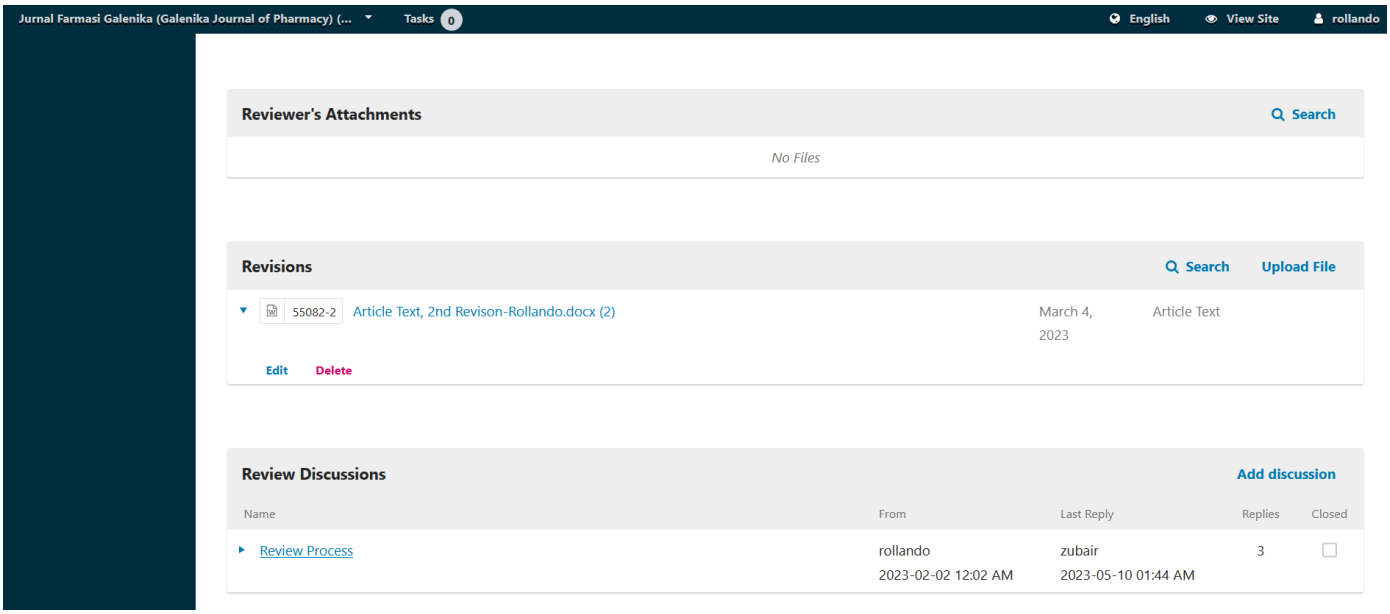
Prof. Apt. M. Sulaiman Zubair, PhD

Editor in Chief

Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)

5. Author mengirimkan hasil perbaikan artikel yang kedua (4-3-2023)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala



6. Editor menyampaikan bahwa artikel diterima untuk diterbitkan (5-6-2023)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

Notifications

[JFG] Editor Decision

2023-06-05 12:35 AM

rollando rollando:

We have reached a decision regarding your submission to Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal), "Computational Study of Momordica Charantia as Natural Antidiabetic".

Our decision is to: Accept Submission

Muhammad Sulaiman Zubair, Ph.D
Tadulako University
sulaiman_zubair80@yahoo.co.id

Reviewer A:
Recommendation: Accept Submission

Reviewer Comment----------

Reviewer B:
Recommendation: Accept Submission

Reviewer Comment

Accepted in the current form

_____

Prof. Apt. M. Sulaiman Zubair, PhD

Editor in Chief

Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

7. Editor menyampaikan bahwa arikel masuk pada proses editing lay out
(11-3-2024)

Dr. apt. Rollando, S.Farm., M.Sc.
Pengajuan ke Lektor Kepala

Notifications

[JFG] Editor Decision

2024-03-11 09:30 AM

Rollando Rollando, Melisa Dwi Chandra, Muhammad Hilmi Aftoni, Windra Swastika:

The editing of your submission, "Molecular Docking and Molecular Dynamic Studies of Secondary Metabolites from Momordica Charantia as Natural Antidiabetic: Studi Penambatan dan Dinamika Molekuler Senyawa Metabolit Sekunder Momordica Charantia sebagai Antidiabetes Alami," is complete. We are now sending it to production.

Submission URL: https://bestjournal.untad.ac.id/index.php/Galenika/authorDashboard/submission/15976

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Prof. Apt. M. Sulaiman Zubair, PhD

Editor in Chief

Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)

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Molecular Docking and Molecular Dynamic Studies of Secondary Metabolites from *Momordica Charantia* as Natural Antidiabetic

(*Studi Penambatan dan Dinamika Molekuler Senyawa Metabolit Sekunder Momordica Charantia sebagai Antidiabetes Alami*)

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ABSTRACT

Background: Diabetes Mellitus is a non-contagious disease characterized by hyperglycemia. Diabetes mellitus occurs when the body cannot receive or use insulin properly. If you already have diabetes, then the patient must take medication continuously because diabetes mellitus is a lifelong disease. Because medicines are quite expensive, alternative ways to cure the disease are needed by consuming traditional medicines, one of which is bitter melon (*Momordica charantia*). **Objectives:** This research aims to predict the secondary metabolite compounds in the bitter melon plant, analyze molecular interactions, and identify compounds that can lower blood sugar levels. **Material and Methods:** 12 compounds from the *Momordica charantia* plant and six proteins (1IR3, 1RHF, 1XU7, 4PNZ, 4YVP, 2NT7) that will be docked using Pyrx and Yasara Dynamics applications. **Results**: From the molecular docking results, three compounds with the highest binding affinity were found in Momordica charantia: momordenol, oleanolic acid, and momordicin. Based on molecular dynamics simulations, these three compounds were stable in their interactions with the six proteins tested, namely 1IR3, 1RHF, 4PNZ, 4YVP, 1XU7, and 2NT7. Momordenol and momordicin showed the most stable interaction profiles. Furthermore, ADMET tests showed that momordenol, oleanolic acid, and momordisin have drug-like characteristics. **Conclusions:** The *Momordica charantia* plant has the potential to act as an antidiabetic agent.

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