


LAMPIRAN

Lampiran 1. Surat Izin Penelitian

	SURAT	No Dokumen	Form-A1
	PERMOHONAN IZIN PENELITIAN PROGRAM STUDI S-1 FARMASI UNIVERSITAS AISYIYAH PALEMBANG	Berlaku Sejak	
		Revisi	000

Hal : Permohonan Izin Penelitian

Kepada Yth
Kabag Laboratorium Terpadu
Universitas 'Aisyiyah Palembang

1	Skripsi
2	PKM/LKTI
3	Penelitian Dosen
4	Luar

Assalamualaikum Wr. Wb.

Sehubungan dengan penelitian kami dalam bidang Kimia Komputasi dengan:
Judul Penelitian : Identifikasi Uraan Antihipertensi Berbasis Tumbuhan dalam Al-Qur'an dan Hadis dengan Metode Structure-based Virtual Screenings (SBSVS)

Nama Pembimbing : 1. Gerry Nugraha, M.Sc., M.Farm
2. Dr. Amrullah, M.Pd.

No	Nama	NIM/NIP/NIK	No. HP
1	<u>Izzaty Parde Muniroh</u>	<u>219820105015</u>	<u>0896 6901 6902</u>
2			
3			
4			
5			

Bermaksud mengajukan izin penelitian di Laboratorium*: Farmasetika Dasar / Teknologi Farmasi / Kimia Farmasi / Biologi Farmasi / Farmakologi / Mikrobiologi / Komputasi Prodi S1 Farmasi Universitas 'Aisyiyah Palembang.

Penelitian tersebut akan kami laksanakan selama: 6 bulan,
yang dihitung dari : 19 03 2025 s.d 19 08 2025

Sebagai bahan pertimbangan, bersama ini dilampirkan lembar pengesahan proposal penelitian. Demikian permohonan kami, atas perhatiannya diucapkan terima kasih.

Palembang, 19 Maret 2025

Mengetahui,
Dosen Pembimbing
Gerry Nugraha, M.Sc., M.Farm

Menyetujui,
Kabag Laboratorium Terpadu

Neni Prandi, S.KM, M. Per

Pemohon
Izzaty Parde Muniroh



Lampiran 2. Lembar Bimbingan



UNISA
UNIVERSITAS 'AISYIYAH PALEMBANG

FAKULTAS KESEHATAN DAN TEKNOLOGI (FKesT)
PROGRAM STUDI :
S1 FARMASI

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FORMULIR BIMBINGAN SKRIPSI

Nama : Izzaty Parla Muniroh
 NIM : 214820103013
 Nama Pembimbing : 1. Dr. Gerry Nugraha, M.Sc., M.Farm
 2. Dr. Amrullah, M.Pd.1
 Judul Skripsi : Identifikasi Ligan Anti-Hipertensi Tumbuhan Dalam Al-Qur'an Dan Hadits Dengan Metode Structure-Based Virtual Screening (SBVS)

No.	Tanggal Konsultasi	Keterangan	Paraf Pembimbing
1	23 mei 2025	Membahas mengenai pembahasan isi skripsi	
2	26 mei 2025	Membahas cara mencari jurnal untuk mempermudah mencari referensi jurnal	
3	27 mei 2025	Evaluasi penulisan Bab I	
4	2 juni 2025	Revisi format penulisan dan isi bab I	
5	3 juni 2025	Revisi isi pembahasan Bab II	
6	4 juni 2025	Revisi tabel bab 4	
7	3 juli 2025	Revisi gambar hasil penelitian	
8	4 juli 2025	Revisi Metode Penelitian	
9	9 juli 2025	Revisi Bab V kesimpulan dan saran	
10	17 juli 2025	Revisi keseluruhan Bab	
11	19 juli 2025	Revisi Bab 2	
12	22 juli 2025	Membahas referensi al-qur'an dan hadits	
13	24 juli 2025	Revisi Bab IV	
14	28 juli 2025	Revisi abstrak	
15	30 juli 2025	Revisi bab I Pembahasan	
16	2 agustus 2025	Revisi bab II Pembahasan	
17	4 agustus 2025	Revisi Kesimpulan	
18	5 agustus 2025	Revisi Lampiran	

Lampiran 3. Hasil Screening Energi Ikatan

000000.4253 | 000013.6100 | 000000000000105.6180 | 000450.97 | LTS0212059 |
 A GLU 162 A TRP 279 A GLN 281 A CYS 352 A HIS 353 A ALA 354 A SER
 355 A GLN 369 A CYS 370 A VAL 380 A HIS 383 A GLU 384 A HIS 387 A
 GLU 411 A ASP 415 A PHE 457 A PHE 460 A LYS 511 A PHE 512 A HIS 513
 A TYR 520 A TYR 523 A SER 526 A PHE 527 |
COc1cc(CC[C@H])(C[C@H])(CCc2ccc(O)c(O)c2)OC(=O)C)OC(=O)C)ccc1O
 0609| 000000.4100 | 000013.5300 | 000000000000120.8867 | 000369.62 |
 LTS0094590 | A GLN 281 A HIS 353 A ALA 354 A SER 355 A VAL 379 A VAL
 380 A HIS 383 A GLU 384 A HIS 387 A GLU 411 A ASP 415 A PHE 457 A PHE
 460 A LYS 511 A PHE 512 A HIS 513 A TYR 520 A TYR 523 A SER 526 A PHE
 527 A GLN 530 |
COc1cc(CC[C@@H])(C[C@@H])(CCc2ccc(O)c(OC)c2)OC(=O)C)OC(=O)C)ccc
 1O
 0609| 000000.4079 | 000013.4600 | 000000000000136.0471 | 000369.40 |
 LTS0094590 | A GLN 281 A HIS 353 A ALA 354 A SER 355 A VAL 379 A VAL
 380 A HIS 383 A GLU 384 A HIS 387 A GLU 411 A ASP 415 A PHE 457 A PHE
 460 A LYS 511 A PHE 512 A HIS 513 A TYR 520 A TYR 523 A SER 526 A PHE
 527 A GLN 530 |
COc1cc(CC[C@@H])(C[C@@H])(CCc2ccc(O)c(OC)c2)OC(=O)C)OC(=O)C)ccc
 1O
 0953| 000000.3667 | 000013.2000 | 000000000000210.9948 | 000435.31 |
 LTS0154111 | A TYR 146 A GLU 162 A TRP 279 A GLN 281 A HIS 353 A ALA
 354 A GLU 376 A VAL 379 A VAL 380 A HIS 383 A GLU 384 A HIS 387 A
 ASP 415 A PHE 457 A PHE 460 A LYS 511 A PHE 512 A HIS 513 A TYR 520
 A TYR 523 A PHE 527 |
C=C1C(=O)O[C@H]2[C@H]1CC[C@@]1(C)C(=O)CC[C@@](C)(C[C@]3(O)
C(=O)O[C@@H]4[C@H]5C(=C)CC[C@H]5C(=C)CC[C@@H]34)[C@H]21
 0068| 000000.4229 | 000013.1100 | 000000000000245.6080 | 000433.11 |
 LTS0011692 | A GLU 162 A GLN 281 A CYS 352 A HIS 353 A ALA 354 A SER
 355 A VAL 380 A HIS 383 A GLU 384 A HIS 387 A GLU 411 A ASP 415 A PHE
 457 A PHE 460 A LYS 511 A PHE 512 A HIS 513 A TYR 520 A TYR 523 A SER
 526 A PHE 527 |
CC(=O)O[C@@H](CCc1ccc(O)c(O)c1)C[C@@H](CCc1ccc(O)c(O)c1)OC(=O)
 C
 0839| 000000.4357 | 000013.0700 | 000000000000262.7622 | 000439.52 |
 LTS0134625 | A TYR 146 A SER 147 A GLN 160 A LEU 161 A GLU 162 A TRP
 279 A VAL 350 A VAL 351 A CYS 352 A HIS 353 A ALA 354 A SER 355 A
 ALA 356 A HIS 383 A GLU 384 A HIS 387 A GLU 411 A LYS 511 A PHE 512
 A HIS 513 A TYR 520 A TYR 523 |
COc1cc(CCC(=O)C[C@H](CCc2ccc(O)c(OC)c2)[S+](=O)([O-])[O-])ccc1O
 0953| 000000.3625 | 000013.0500 | 000000000000271.7835 | 000434.26 |
 LTS0154111 | A TYR 146 A GLU 162 A TRP 279 A GLN 281 A HIS 353 A ALA
 354 A GLU 376 A VAL 379 A VAL 380 A HIS 383 A GLU 384 A HIS 387 A
 ASP 415 A PHE 457 A PHE 460 A LYS 511 A PHE 512 A HIS 513 A TYR 520

A TYR 523 A PHE 527 |
C=C1C(=O)O[C@H]2[C@H]1CC[C@@]1(C)C(=O)CC[C@@](C)(C[C@]3(O)
C(=O)O[C@@H]4[C@H]5C(=C)CC[C@H]5C(=C)CC[C@@H]34)[C@H]21
0963| 000000.4203 | 000013.0300 | 00000000000281.1146 | 000430.60 |
LTS0155465 | A GLN 281 A HIS 353 A ALA 354 A SER 355 A ALA 356 A HIS
383 A GLU 384 A HIS 387 A TYR 390 A PHE 391 A TYR 394 A ARG 402 A
GLU 403 A GLY 404 A HIS 410 A GLU 411 A PHE 457 A LYS 511 A PHE 512
A HIS 513 A TYR 520 A TYR 523 |

Lampiran 4. Hasil nilai RMSD (*Rood Mean Square Devination*)

8.3675	1.3288	1.3087
8.3359	1.3275	1.3084
8.2869	1.3252	1.3081
8.2717	1.3242	1.3065
8.2263	1.3226	1.3065
8.2225	1.3223	1.306
3.1575	1.3216	1.3056
2.8988	1.3216	1.3055
1.9992	1.3213	1.3053
1.7578	1.3208	1.3052
1.691	1.3191	1.305
1.6887	1.319	1.3048
1.6785	1.3188	1.3047
1.6248	1.3186	1.3045
1.6132	1.3182	1.3044
1.6113	1.3181	1.3042
1.6088	1.318	1.3042
1.6083	1.3176	1.3039
1.6001	1.3175	1.3032
1.5993	1.3166	1.3031
1.5988	1.3165	1.303
1.5945	1.3157	1.3029
1.5921	1.3147	1.3029
1.5886	1.3146	1.3028
1.5878	1.3142	1.3022
1.5744	1.3142	1.3019
1.5571	1.314	1.3012
1.4103	1.3138	1.3011
1.3602	1.3131	1.3006
1.3483	1.3131	1.3006
1.3449	1.3128	1.3002
1.3408	1.3127	1.3001
1.34	1.3117	1.3
1.3384	1.3117	1.2997
1.338	1.3114	1.2997
1.3329	1.3114	1.2995
1.3315	1.3113	1.2992
1.3308	1.3113	1.2989
1.3307	1.3101	1.2987
1.329	1.3092	1.2986

Lampiran 5. Perintah dari *target_perp.mcr*

```
#target preparation
LoadPdb (MacroDir)\op_1o8600179.pdb
SplitObj 1
#DelObj 3
NiceOriAll
Cell Auto,Extension=5,Shape=Cuboid,Obj 2
FixAll
ForceField NOVA,SetPar=Yes
Boundary Wall
FreeAll
SaveYOb 2,/home/al/yasara/00_2021/izzaty/02_redock/1o86_ligand.yob
SaveYob 2,/home/al/yasara/00_2021/izzaty/02_redock/1o86_ligandref.yob
FixAll
DelObj 2
SaveSce (MacroDir)\1o86_receptor.sce
#Clear
```

Lampiran 6. Perintah *dock_run1000x.mcr*.

```

# YASARA MACRO
# TOPIC: 5. Structure prediction
# TITLE: Docking a ligand to a receptor
# REQUIRES: Structure
# AUTHOR: Elmar Krieger
# LICENSE: GPL
# DESCRIPTION: This macro predicts the structure of a ligand-receptor complex.
It can also continue a docking run that got interrupted. An analysis log file is written
at the end.
#
# Parameter section - adjust as needed, but NOTE that some changes only take
effect
# if you start an entirely new docking job, not if you continue an existing one.
#
=====
=====
# Energy minimization experiment completed after 765 steps. Final energy is -
20568.574 kJ/mol.
# MODIFIED YASARA MACRO by Roy Gunawan Wicaksono (11 Oct 2019)
# DESCRIPTION: This macro re-dock 1000 times ligand to its receptor to examine
the applicability of the receptor for virtual screening
Processors CPUThreads=10,GPU=1
Antialias 0
Console Off
method='AutoDockLGA'
#method='VINA'
runs=5
rmsdmin=5.0
rigid=0
flexres=""
calcspread=1
pdbsaved=0
ForceField AMBER03
# Normally no change required below this point
# =====
# Sanity checks
if MacroTarget=="
#MacroTarget
/home/al/yasara/00_lotus2024/03_redock/4yay_receptor.sce,Remove=FromUnder
score
RaiseError "This macro requires a target. Either edit the macro file or click Options
> Macro > Set target to choose a target structure" if runs>99

```

Lampiran 7. Perangkat Lunak YASARA-Structure

YASARA - Yet Another Scientific Artificial Reality Application

File Edit Simulation Analyze View Effects Options Window Help

ATOMPROPERTIES

Number:
Name:
Element:
Occupancy: % BFactor:
Residue:
Object:

Position: X = 000000.00000 Å
Y = 000000.00000 Å
Z = 000000.00000 Å

Speed: X = 0000000000 m/s
Y = 0000000000 m/s
Z = 0000000000 m/s
Total = 0000000000 m/s

Active X = 0000000000 fN
Forces Y = 0000000000 fN
Z = 0000000000 fN
Total = 0000000000 fN

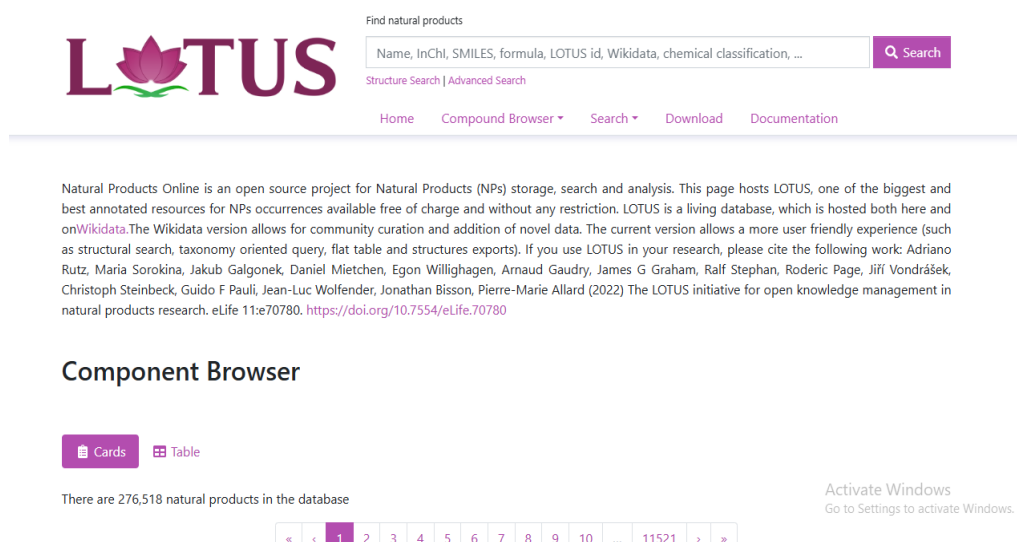
Bonds:
1) Type to ---- (-) Length ---- Å
2) Type to ---- (-) Length ---- Å
3) Type to ---- (-) Length ---- Å
4) Type to ---- (-) Length ---- Å

Marked Distance: ---- Å
Marked Angle: ---- °
Marked Dihedral: ---- °

SCENE CONTENT

Obj	Name	Vis	Act	Atom
1	-----	No	No	-----
2	-----	No	No	-----
3	-----	No	No	-----
4	-----	No	No	-----
5	-----	No	No	-----
6	-----	No	No	-----
7	-----	No	No	-----
8	-----	No	No	-----
9	-----	No	No	-----
10	-----	No	No	-----

Lampiran 8. Lotus Natural Product (laman lotus yang sebagai sumber struktur senyawa bahan alam)



Find natural products

LOTUS

Name, InChI, SMILES, formula, LOTUS id, Wikidata, chemical classification, ... Search

Structure Search | Advanced Search

Home Compound Browser Search Download Documentation

Natural Products Online is an open source project for Natural Products (NPs) storage, search and analysis. This page hosts LOTUS, one of the biggest and best annotated resources for NPs occurrences available free of charge and without any restriction. LOTUS is a living database, which is hosted both here and on Wikidata. The Wikidata version allows for community curation and addition of novel data. The current version allows a more user friendly experience (such as structural search, taxonomy oriented query, flat table and structures exports). If you use LOTUS in your research, please cite the following work: Adriano Rutz, Maria Sorokina, Jakub Galgonek, Daniel Mietchen, Egon Willighagen, Arnaud Gaudry, James G Graham, Ralf Stephan, Roderic Page, Jiří Vondrášek, Christoph Steinbeck, Guido F Pauli, Jean-Luc Wolfender, Jonathan Bisson, Pierre-Marie Allard (2022) The LOTUS initiative for open knowledge management in natural products research. eLife 11:e70780. <https://doi.org/10.7554/eLife.70780>

Component Browser

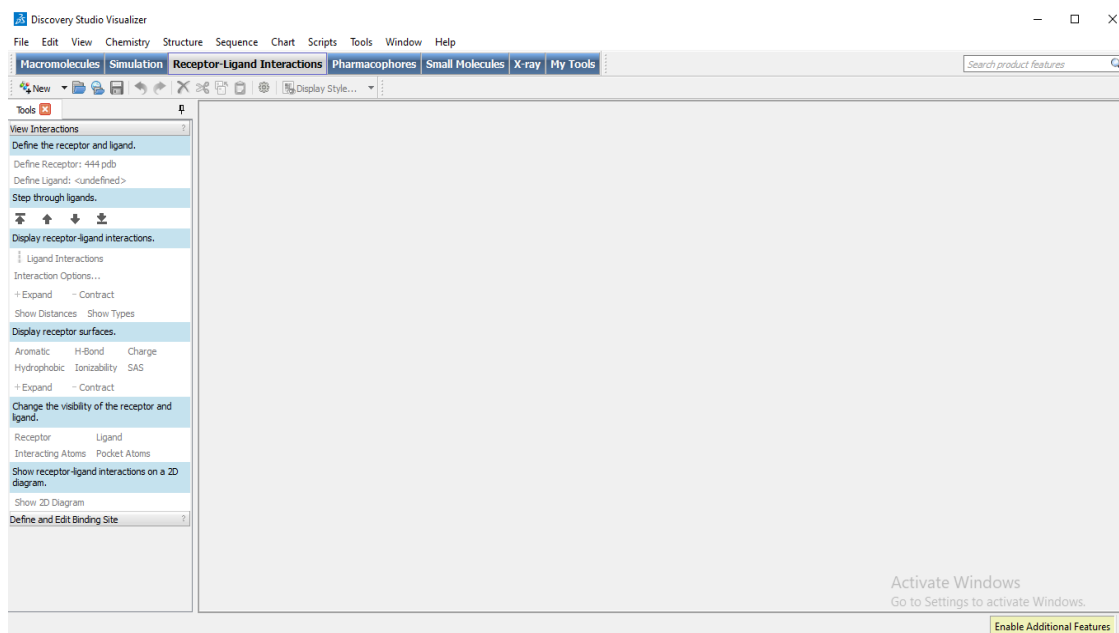
Cards Table

There are 276,518 natural products in the database


Activate Windows
Go to Settings to activate Windows.

<< 1 2 3 4 5 6 7 8 9 10 ... 11521 >>

Lampiran 9. Perangkat Lunak *Discovery Visualizer*



Lampiran 10. Pernyataan Selesai Revisi Skripsi



**FAKULTAS ILMU KESEHATAN DAN TEKNOLOGI
'AISYIYAH PALEMBANG
PROGRAM STUDI SI FARMASI**

Jl. Kol. H. Burlian –Lr. M. Husin No. 907 RT. 12/RW. 04 Kel. Karya Baru
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www.unisa-palembang.ac.id farmasi.aisyiyah@gmail.com

بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ





**FORMULIR
PERNYATAAN SELESAI REVISI NASKAH SKRIPSI*)
(S-06)**

Yang bertandatangan dibawah ini, tim penguji ~~Skripsi 1/~~ Skripsi 2*):

Nama Mahasiswa : Izzaty Parda Muniroh
NIM : 214820103013
Judul Penelitian : Identifikasi Ligan Anti-Hipertensi Berbasis Bahan Alam yang Disebutkan Dalam Al-Qur'an Dan Hadits Dengan Metode *Structure-Based Virtual Screening* (SBVS) Pada Target Reseptor ACE

Pembimbing 1 : Dr. Gerry Nugraha, M.Sc., M.Farm.
Pembimbing 2 : Dr. Amrullah, M.Pd.I.
Tanggal Ujian : 14 Agustus 2025

Menerangkan bahwa naskah ~~Proposal/~~ Skripsi*) telah selesai direvisi oleh tim penguji.

Nama	Tanda Tangan	Tanggal
1. Dr. Gerry Nugraha, M.Sc., M.Farm.		01/2025/10
2. Dr. Amrullah, M.Pd.I.		28/2025/09
3. Deden Mula Saputra, S.Th.I., M.Ud.		01/2025/10
4. Intan Trisakti, M.Farm.		27/25/9

*) : Coret yang tidak perlu.