

DAFTAR PUSTAKA

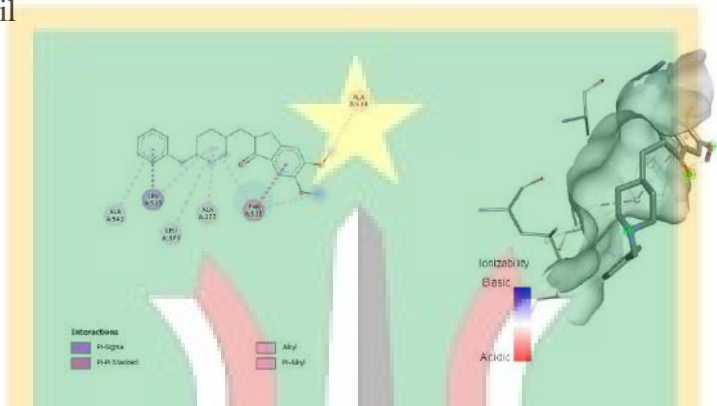
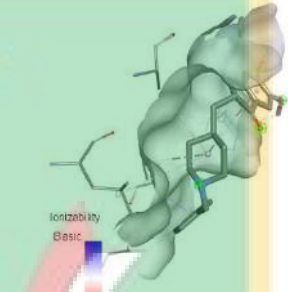

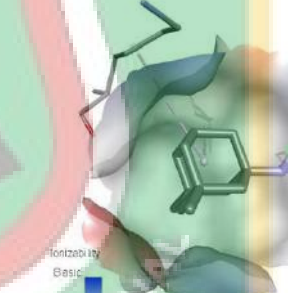
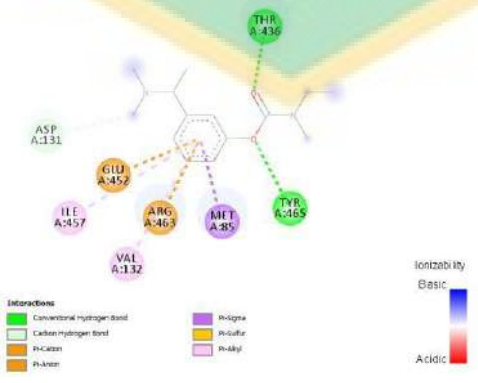
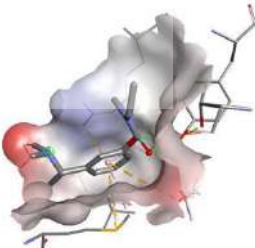
- Abdillah MY, Amalia Y, Novita D. 2023. Studi *In Silico* : Potensi senyawa aktif daun serai (*Cymbopogon citratus*) sebagai obat herbal antiinflamasi dengan mekanisme aktivasi COX-1 dan penghambatan COX-2. *Jurnal kedokteran komunitas (Journal of community medicine)* 11
- Ananto AD, Muliastari H, Hamdin CD. 2020. Studi *In Silico* bioaktivitas antikanker senyawa aktif dalam minyak biji buah wali (*Brucea javanica* (L.) Merr). *Sasambo journal of pharmacy* 1: 26-9
- Adelina R. 2014. Uji *molecular docking* Annomuricin E dan Muricapentocin pada aktivitas antiproliferasi (*Molecular docking studies of Annomuricin E and Muricapentocin on antiproliferation activity*). *Jurnal ilmu kefarmasian Indonesia* 12: 32-6
- Aparoy P, Kumar Reddy K, Reddanna P. 2012. Structure and ligand based drug design strategies in the development of novel 5-LOX inhibitors. *Current medicinal chemistry* 19: 3763-78
- Apriali KD, Triana E, Farhani MI, *et al.* 2022. Studi penambatan molekul dan prediksi ADMET senyawa metabolit sekunder tanaman kelor (*Moringa oleifera* L.) sebagai inhibitor BACE 1 pada penyakit Alzheimer . *Fitofarmaka : Jurnal ilmiah farmasi* 12: 58-67
- Bachurin SO, Bovina EV, Ustyugov AA. 2017. Drugs in clinical trials for Alzheimer's disease: the major trends. *Medicinal research reviews* 37: 1186-225
- Banerjee P, Eckert AO, Schrey AK, *et al.* 2018. ProTox-II: a webserver for the prediction of toxicity of chemicals. *Nucleic acids research* 46: W257-W63
- Cava C, Bertoli G, Castiglioni I. 2020. *In Silico* discovery of candidate drugs against Covid-19. *Viruses* 12: 404
- Coimbra JR, Marques DF, Baptista SJ, *et al.* 2018. Highlights in BACE1 inhibitors for Alzheimer's disease treatment. *Frontiers in chemistry* 6: 178
- Cortes-Torres AG, López-Castillo GN, Marín-Torres JL, *et al.* 2023. *Cymbopogon citratus* essential oil: Extraction, GC-MS, phytochemical analysis, antioxidant activity, and *In Silico* Molecular docking protein targets related to CNS. *Current issues in molecular biology* 45: 5164-79
- Das, B., & Yan, R. 2017. Role of BACE1 in Alzheimer's synaptic function translational neurodegeneration, 6(1), 4-11. <https://doi.org/10.1186/s40035-017-0093-5>

- Daina A, Michielin O, Zoete V. 2017. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Scientific reports* 7: 1-13
- Dos Santos RN, Ferreira LG, Andricopulo AD. 2018. Practices *moleculer docking* and structure-based virtual screening. *Computational drug discovery and design*: 31-50
- Fan, J., Fu, A., & Zhang, L. 2019. Progress in *molecular docking*. *Quantitative Biology*, 7, 83-89.
- Holtzman DM, Morris JC, Goate AM. 2011. Alzheimer's disease: the challenge of the second century. *Science translational medicine* 3: 77sr1-sr1
- Jia J, Wei C, Jia L, *et al.* 2017. Efficacy and safety of donepezil in chinese patients with severe alzheimer's disease: A randomized controlled trial. *Journal of Alzheimer's disease* 56: 1495-504
- Kitphati, W., Wattanakamolkul, K., *et al.* 2012, Anticholinesterase of essential oil and their constituents from Thai medicinal plants purified and selular enzymes, *JAASP*, 1: 58 – 6.
- Levita J, Mustarichie R. 2012. Pemodelan molekul dalam kimia medisinal. *Yogyakarta: Graha ilmu*
- Liu Y-Y, Feng X-Y, Jia W-Q, *et al.* 2019. Identification of novel PI3K δ inhibitors by *molecular docking*, ADMET prediction and molecular dynamics simulations. *Computational biology and chemistry* 78: 190-204
- Makatita FA. 2020. Riset *In Silico* dalam pengembangan sains di bidang pendidikan, studi kasus: analisis potensi cendana sebagai agen anti-aging. *Jurnal ABDI (Sosial, budaya dan Sains)* 2
- Meng X-Y, Zhang H-X, Mezei M, *et al.* 2011. *Molecular docking* : a powerful approach for structure-based drug discovery. *Current computer-aided drug design* 7: 146-57
- Novian DR, Ikhwan AZN, Winarso A. 2019. Uji farmakodinamik, drug-likeness, farmakokinetik dan interaksi senyawa aktif kayu ular (*Strychnos lucida*) sebagai inhibitor *Plasmodium falciparum* secara *In Silico*. *Jurnal Veteriner Nusantara* 2: 70-8
- Moroy G, Martiny VY, Vayer P, *et al.* 2012. Toward *In Silico* structure-based ADMET prediction in drug discovery. *Drug discovery today* 17: 44-55
- Pratama MRF. 2016. Studi penambatan molekul senyawa turunan kuinolin terhadap reseptor Estrogen- α (*Molecular docking Study of Quinoline Derivatives Towards Estrogen- α Receptor*). *Jurnal Surya Medika* 2

- Reubun YTA, Kumala S, Setyahadi S, *et al.* 2020. Penghambatan enzim *Asetilkolinesterase* dari ekstrak herba pegagan (*Centella asiatica* (L.) Urb), ekstrak daun kelor (*Moringa oleifera* Lam.) dan kombinasinya. *Jurnal farmasi Indonesia (Pharmaceutical journal of Indonesia)* 17: 451-8
- Ruswanto, R. (2015). Molecular penambatan molekul empat turunan isonicotinohydrazide pada mycobacterium tuberculosis enoyl-acyl carrier protein reductase (InhA). *Jurnal kesehatan bakti tunas husada: Jurnal ilmu-ilmu keperawatan, analisis kesehatan dan farmasi*, 13(1).
- Suhud, F. 2015. Uji aktivitas *in-silico* senyawa baru 1-benzil-3-benzoilurea induk dan tersubstitusi sebagai agen antiproliferatif. *Jurnal farmasi Indonesia*, 7(4), 245-251.
- Susanti N, Saputra D, Hendrayati P, *et al.* 2019. Penambatan molekul likopen sebagai antiosteoporosis secara *In Silico*. *Chimera* 1
- Vargas JAR, Lopez AG, Piñol MC, *et al.* 2018. *Molecular docking* study on the interaction between 2-substituted-4, 5-difuryl Imidazoles with different protein target for antileishmanial activity. *Journal of applied pharmaceutical science* 8: 014-22
- Verawati A, Anam K, Kusri D. 2013. Identifikasi kandungan kimia ekstrak etanol serai bumbu (*Andropogon citratus* DC) dan uji efektivitas repelen terhadap nyamuk *Aedes aegypti*. *Jurnal sains dan matematika* 21: 20-4
- Wardaniati I, Herli MA. 2018. Studi penambatan molekul senyawa golongan Flavonol sebagai antibakteri. *JOPS (Journal of pharmacy and science)* 1: 20-7
- Yang H, Sun L, Li W, *et al.* 2018. *In Silico* prediction of chemical toxicity for drug design using machine learning methods and structural alerts. *Frontiers in chemistry* 6: 30
- WHO. 2021. Dementia. <https://www.who.int/news-room/fact-sheets/detail/dementia>

Lampiran

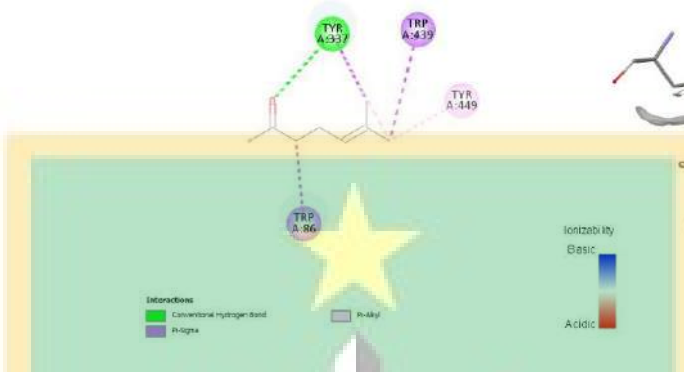
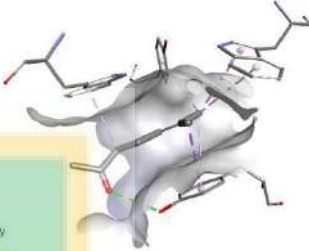
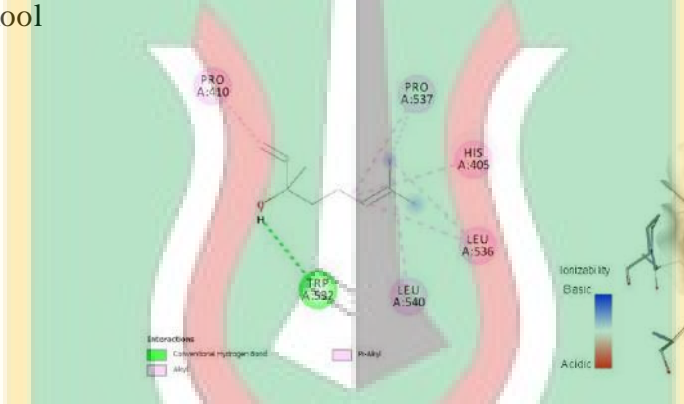
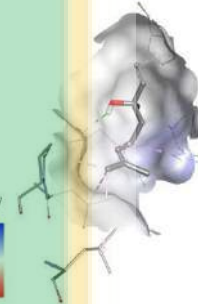
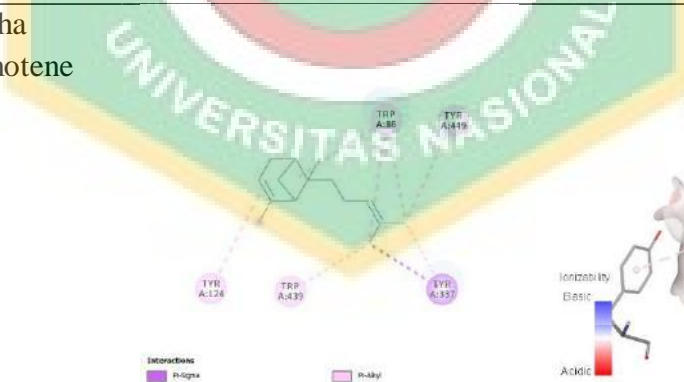
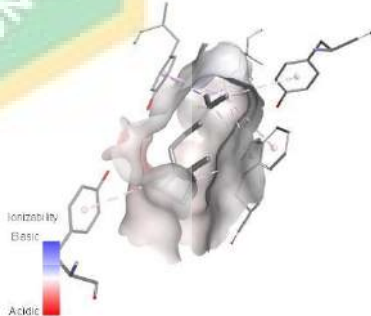
Tabel Lampiran 1. Interaksi Diagram 2D dan Visualisasi 3D antar drug target 4BDT dengan senyawa pembanding

No	Senyawa	Interaksi 2D	visualisasi 3D
1	Donepezil		
2	Memantine		
3	Rivastigmine		

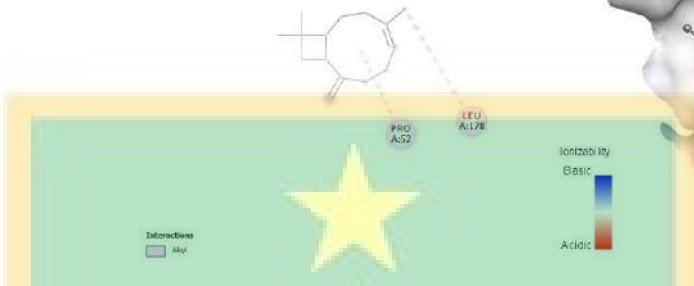
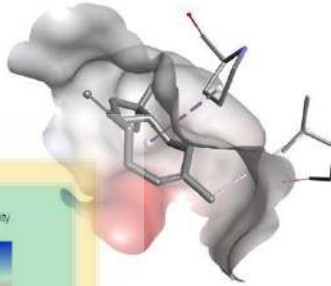
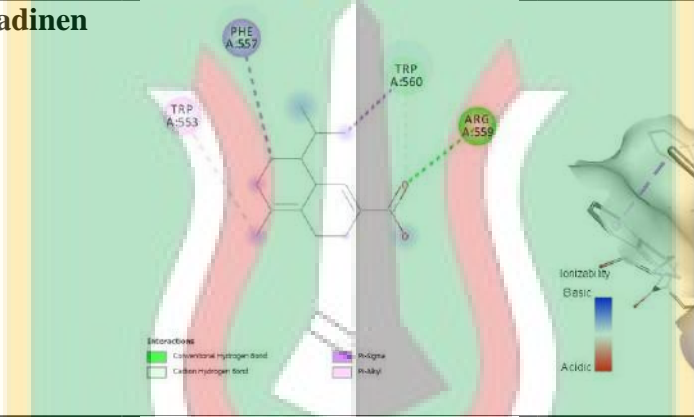
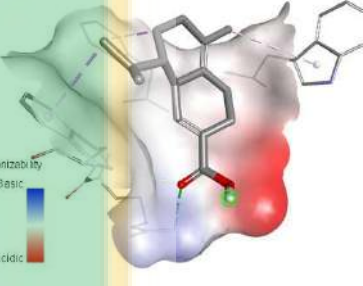
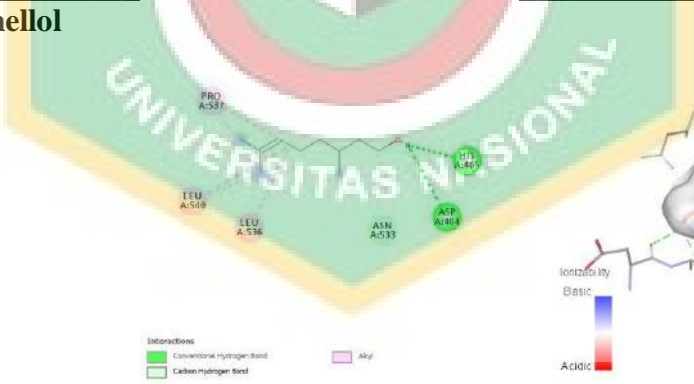
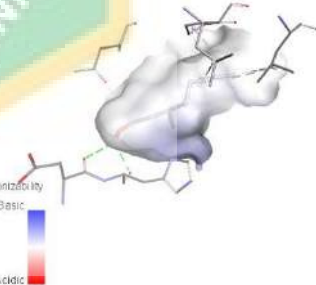
Tabel Lampiran 2. Interaksi Diagram 2D dan Visualisasi 3D antar drug target 3L5D dengan senyawa pembanding

No	Senyawa	Interaksi 2D	Visualisasi 3D
1	Donepezil		
2	Memantine		
3	Rivastigmine		

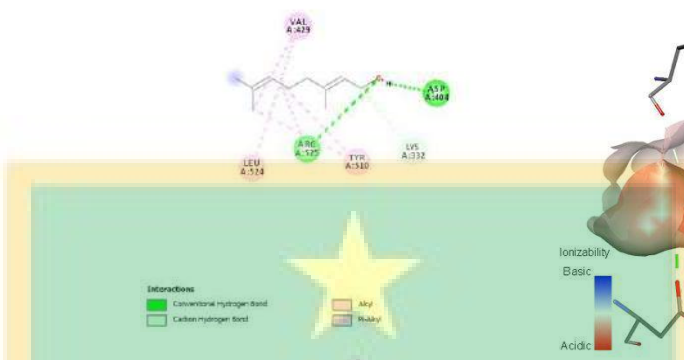
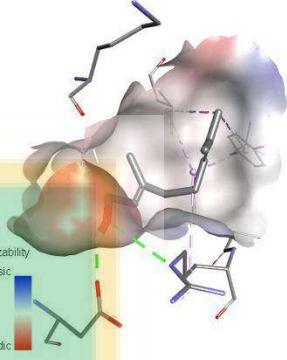
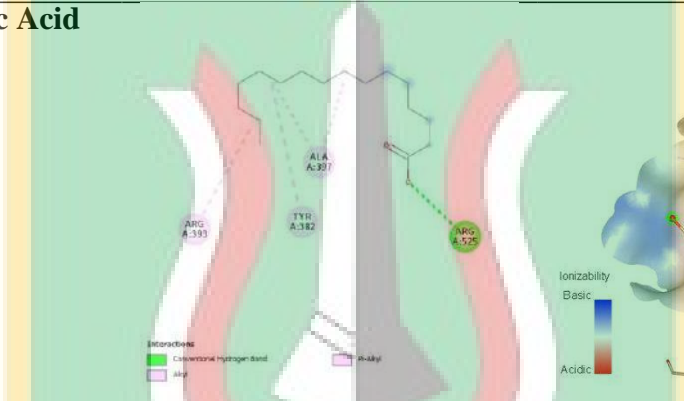
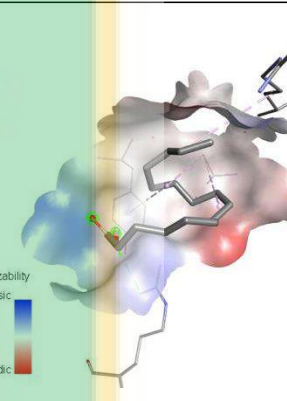
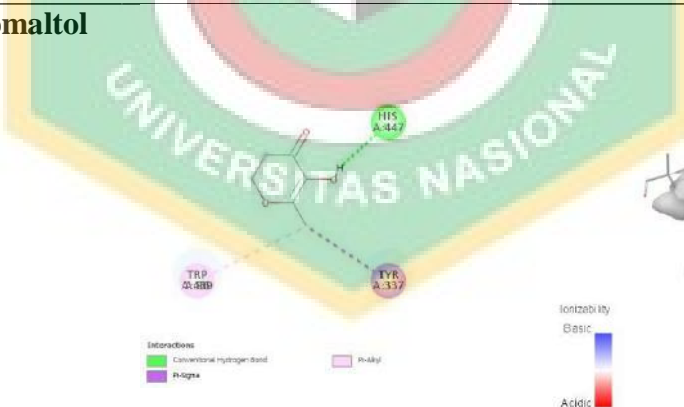
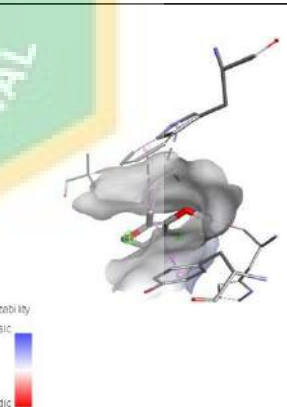
Tabel Lampiran 3. Interaksi Diagram 2D dan Visualisasi 3D antar drag target 4BDT dengan senyawa ligan

No	Senyawa	Interaksi 2D	visualisasi 3D
1	Methylheptenon		
2	Linalool		
3	Alpha Bergamotene		

Tabel Lampiran 3 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
4	Isocaryophyllen		
5	Delta-Cadinen		
6	Citronellol		

Tabel Lampiran 3 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
7	Geraniol		
8	Palmitic Acid		
9	Dihydromaltol		

Tabel Lampiran 3 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
10	Coumaran		
11	Benzoic Acid		
12	Ethyl Linoleate		

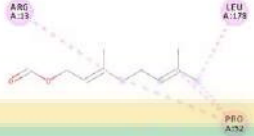
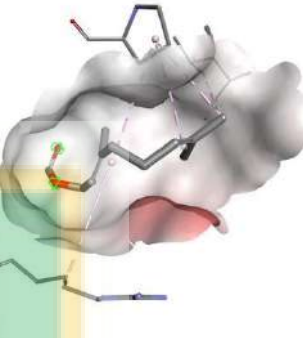
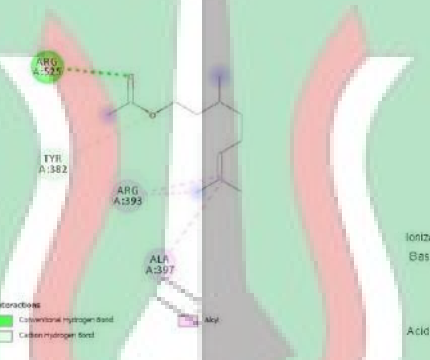
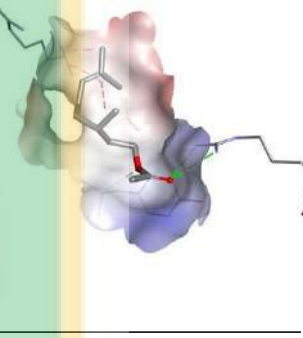

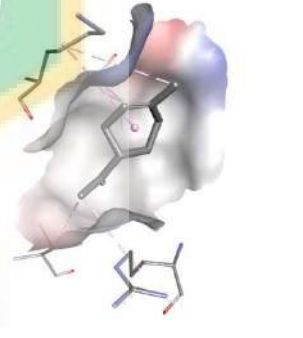
Tabel Lampiran 3 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
13	Hidroxymethylfurfural		
14	Hexadecanol		
15	Sabinene		

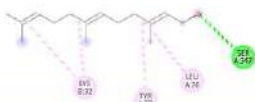
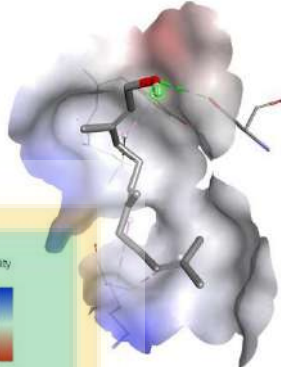
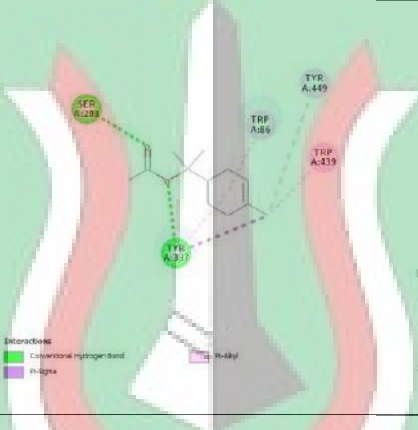
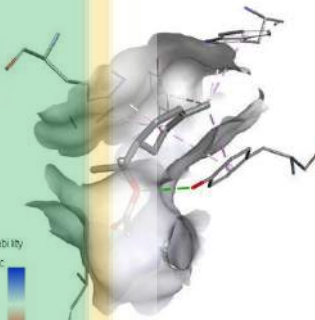


Tabel Lampiran 3 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
16	Myrene	<p>2D interaction diagram for Myrene. The molecule is shown in a stick representation with dashed lines indicating interactions with residues LYS B:136, ALA A:304, and MET A:276. A legend indicates interactions: Pi-Sulfur (yellow box) and Pi-Alky (pink box). A yellow star is present in the center of the diagram.</p>	<p>3D visualization of Myrene bound to a protein surface. The protein surface is shown with an electrostatic potential map (red for acidic, blue for basic). Myrene is shown in a stick representation within the binding pocket.</p>
17	Borneol	<p>2D interaction diagram for Borneol. The molecule is shown in a stick representation with dashed lines indicating interactions with residues GLU B:172, MET A:276, LYS B:136, and ALA A:304. A legend indicates interactions: Conventional hydrogen bond (green box) and Alky (pink box).</p>	<p>3D visualization of Borneol bound to a protein surface. The protein surface is shown with an electrostatic potential map. Borneol is shown in a stick representation within the binding pocket.</p>
18	Bornyl Acetate	<p>2D interaction diagram for Bornyl Acetate. The molecule is shown in a stick representation with dashed lines indicating interactions with residues VAL A:408, ARG A:525, VAL A:429, VAL A:530, TYR A:510, and ARG A:523. A legend indicates interactions: Conventional hydrogen bond (green box) and Alky (pink box).</p>	<p>3D visualization of Bornyl Acetate bound to a protein surface. The protein surface is shown with an electrostatic potential map. Bornyl Acetate is shown in a stick representation within the binding pocket.</p>

Tabel Lampiran 3 Lanjutan

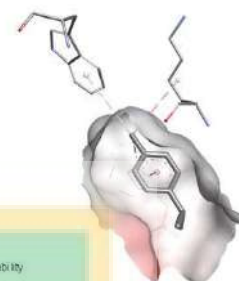
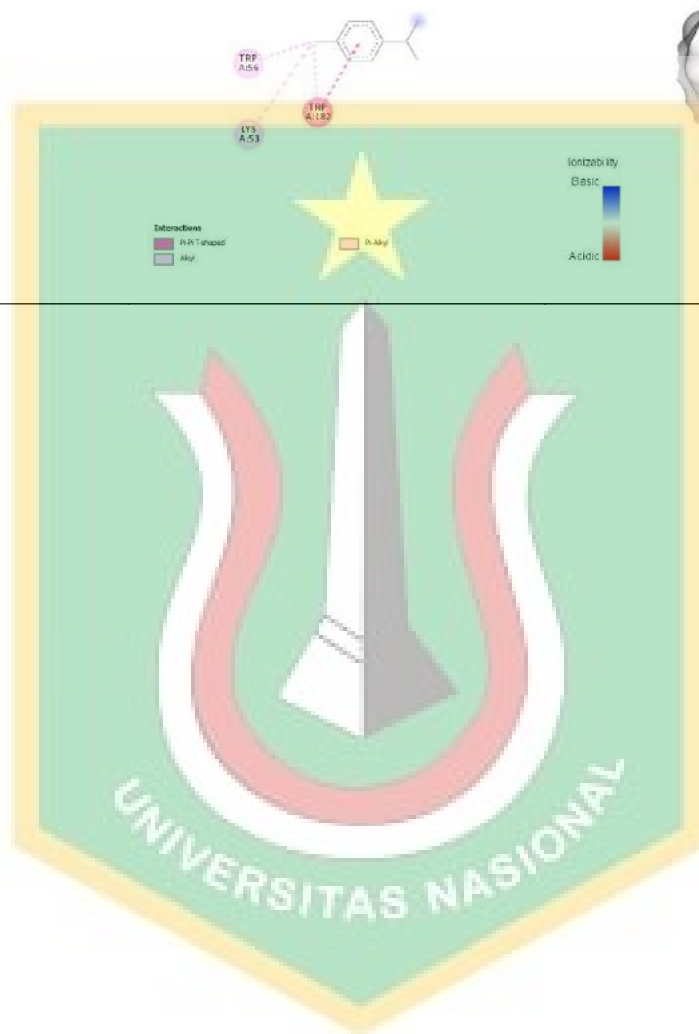
No	Senyawa	Interaksi 2D	visualisasi 3D
19	Geranyl Formate		
20	Citronellyl Acetate		
21	Dipentene		

Tabel Lampiran 3 Lanjutan

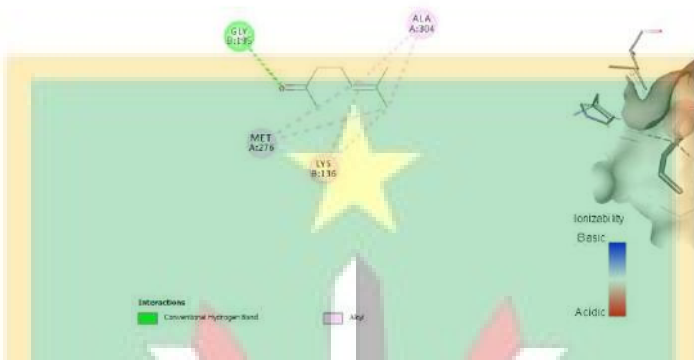
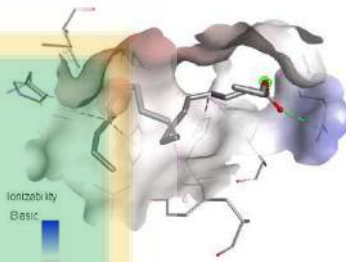
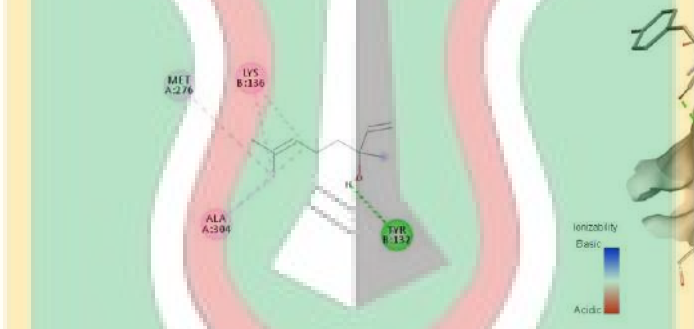
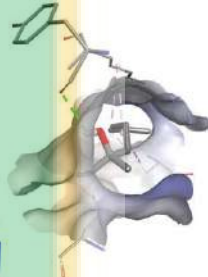

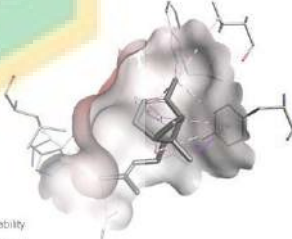
No	Senyawa	Interaksi 2D	visualisasi 3D
22	Farnesol		
23	Alpha Terpinyl Acetate		
24	Beta-Phellandrene		

Tabel Lampiran 3 Lanjutan

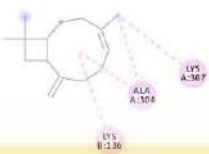
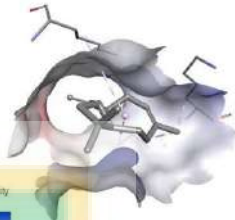
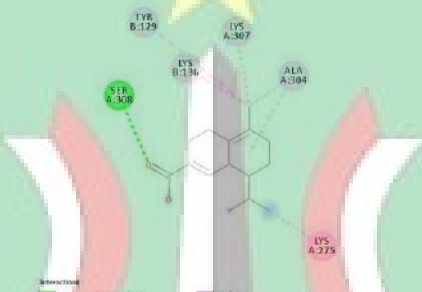
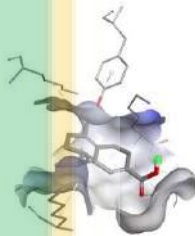
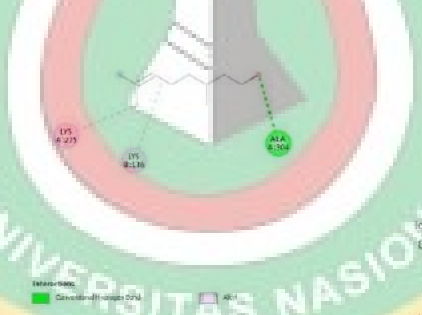
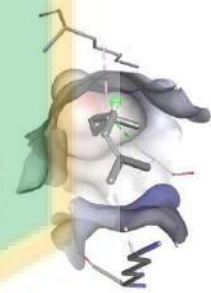
No	Senyawa	Interaksi 2D	visualisasi 3D
25	P-Cymene		



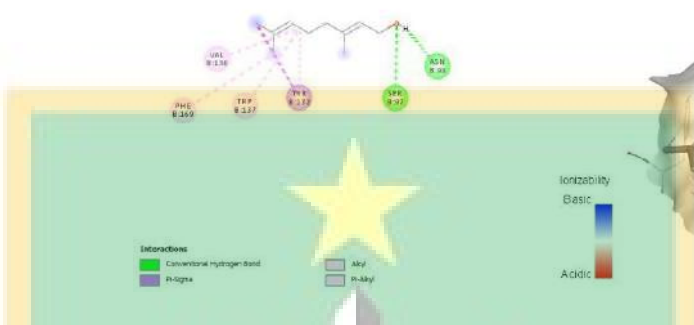
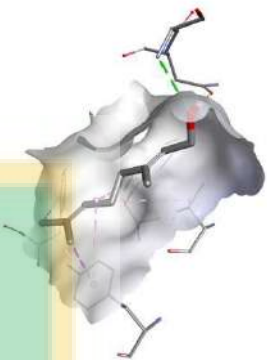
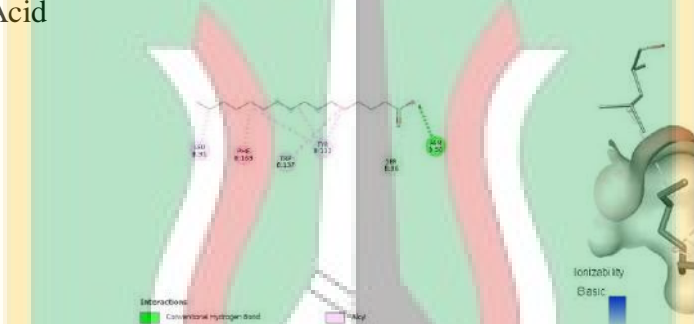
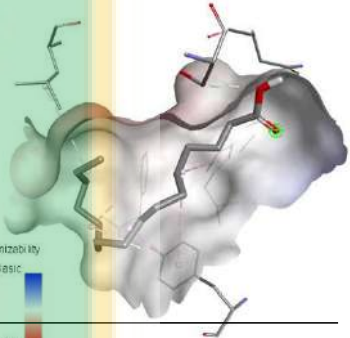

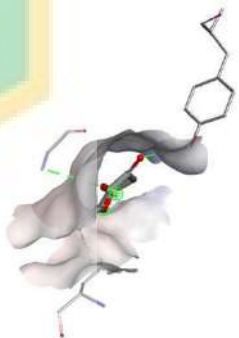
Tabel Lampiran 4. Interaksi Diagram 2D dan Visualisasi 3D antar drag target 3L5D dengan senyawa ligan

No	Senyawa	Interaksi 2D	visualisasi 3D
1	Methylheptenon		
2	Linalool		
3	Alpha Bergamotene		

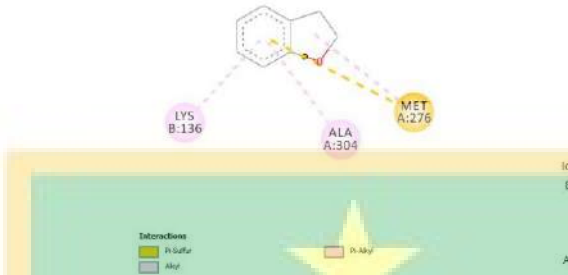
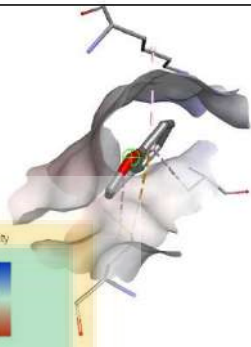
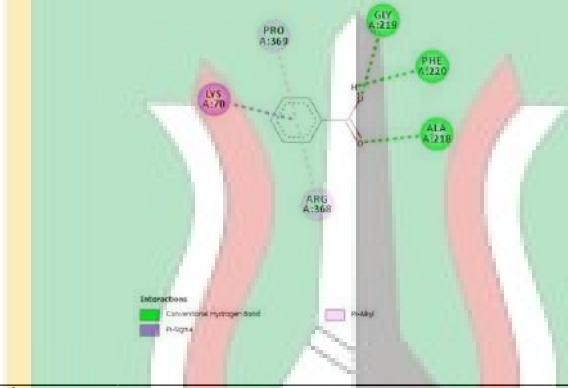
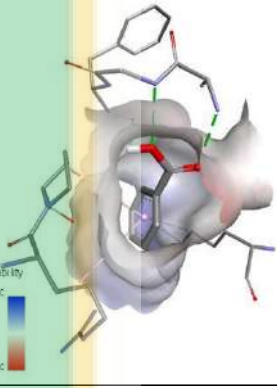
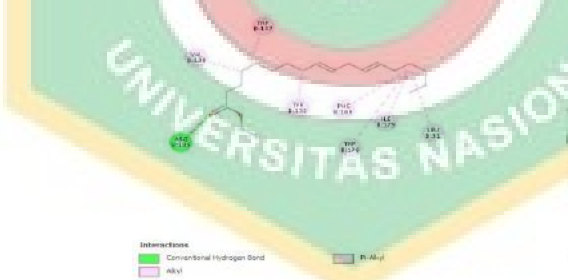
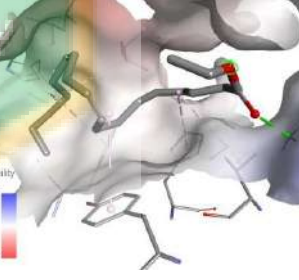
Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
4	Isocaryophyllen		
5	Delta-Cadinen		
6	Citronellol		

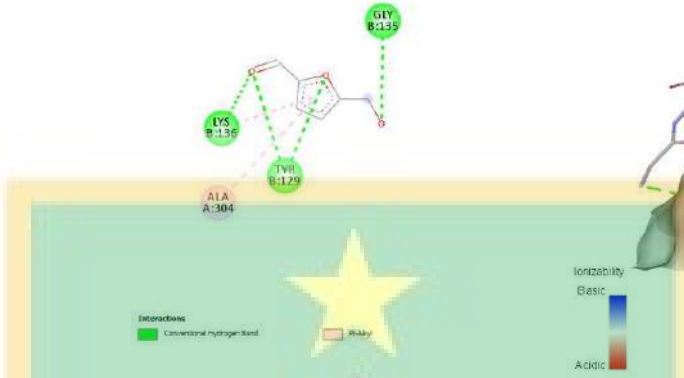
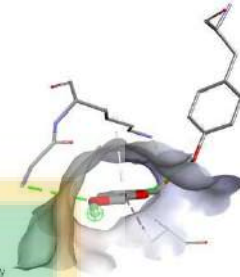
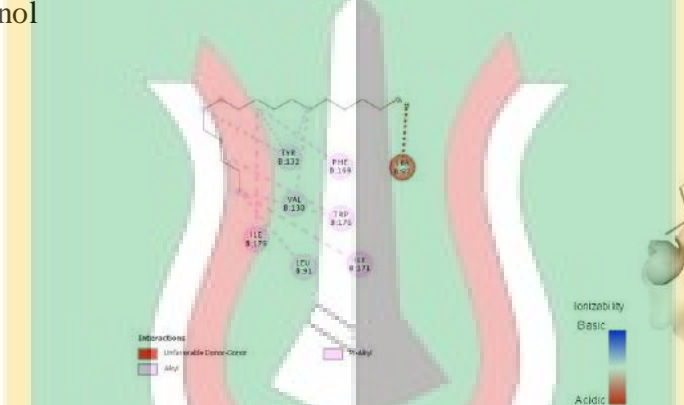
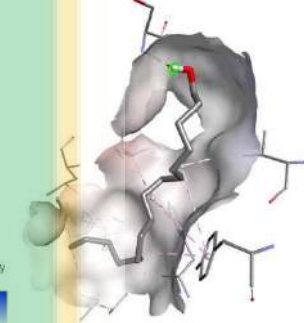


Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
7	Geraniol		
8	Palmitic Acid		
9	Dihydromaltol		

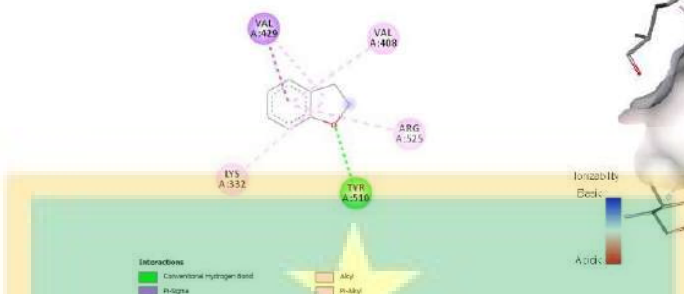
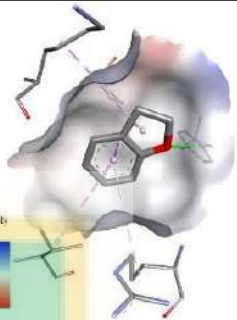
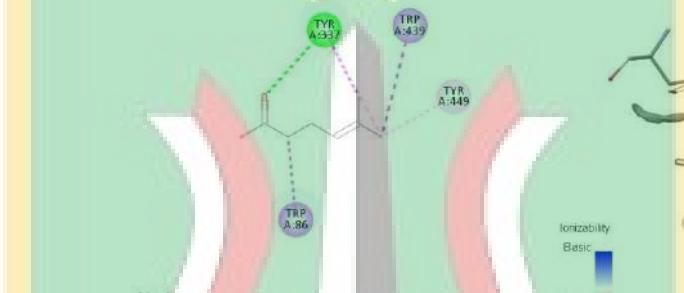
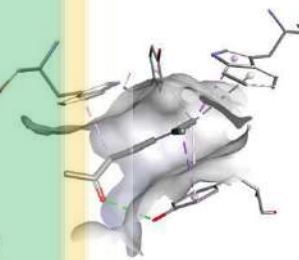

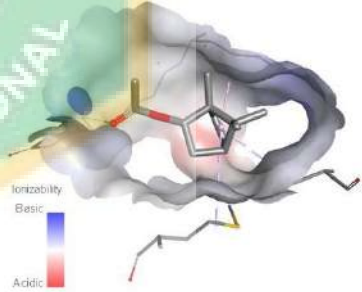
Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
10	Coumaran		
11	Benzoic Acid		
12	Ethyl Linoleate		

Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
13	Hidroxymethylfurfural	 <p>Interaksi: Conventional hydrogen bond, Alkyl</p> <p>Ionizability: Basic, Acidic</p>	
14	Hexadecanol	 <p>Interaksi: Hydrophobic Contact, Alkyl</p> <p>Ionizability: Basic, Acidic</p>	
15	Sabinene	 <p>Interaksi: Alkyl</p> <p>Ionizability: Basic, Acidic</p>	

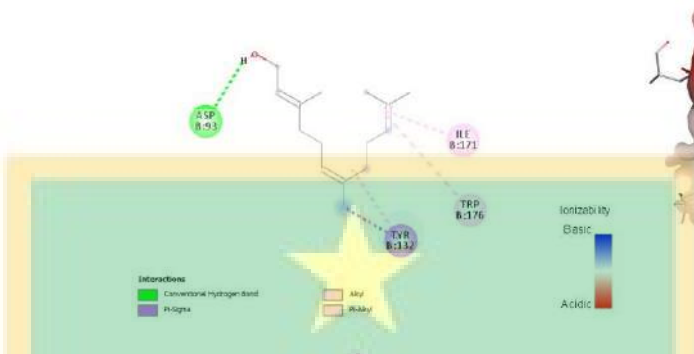
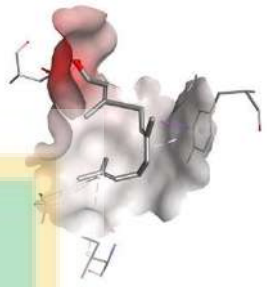
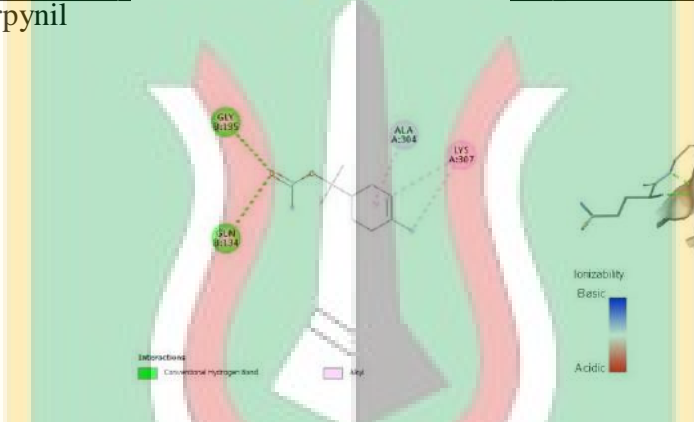
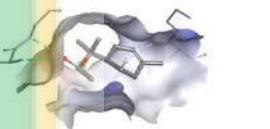
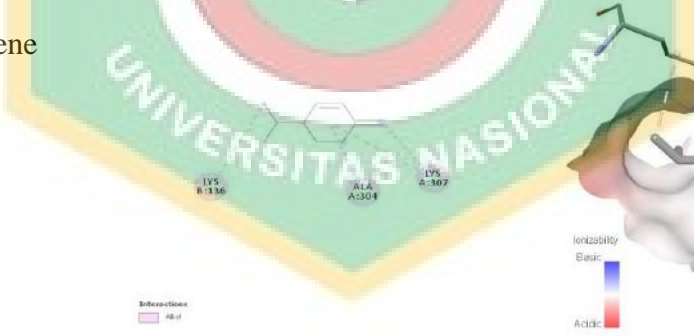
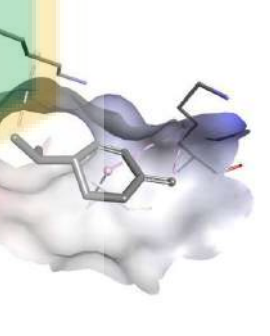
Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
16	Myrene		
17	Borneol		
18	Bornyl Acetate		

Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
19	Geranyl Formate		
20	Citronellyl Acetate		
21	Dipentene		

Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
22	Farnesol		
23	Alpha Terpinyl Acetate		
24	Beta-Phellandrene		

Tabel Lampiran 4 Lanjutan

No	Senyawa	Interaksi 2D	visualisasi 3D
25	P-Cymene		



INTERAKSI SENYAWA-SENYAWA BIOAKTIF DALAM TANAMAN SEREH DAPUR (*Cymbopogon citratus*) TERHADAP RESEPTOR ACETYLHOLINESTERASE DAN BACE 1 : STUDI IN SILICO UNTUK MENEMUKAN OBAT PENYAKIT ALZHEIMER

ORIGINALITY REPORT

24 %

24%

4%

12%

SIMILARITY INDEX

INTERNET SOURCES

PUBLICATIONS

STUDENT PAPERS

PRIMARY SOURCES



6

repository.unas.ac.id
Internet Source

1%



7

core.ac.uk
Internet Source

1%

8

ejournals.stfm.ac.id
Internet Source

1%



