DAFTAR PUSTAKA

Aminuddin, A., Sima, Y., Izza, N.C., Lalla, N.S.N., and Arda, D., 2023. Edukasi Kesehatan Tentang Penyakit Diabetes Melitus bagi Masyarakat. *Abdimas Polsaka: Jurnal Pengabdian Kepada Masyarakat*. Vol. 2. No. 1.

Aroyehun, A.Q.B., Razak, S.A., Palaniveloo, K., Nagappan, T., Rahmah, N.S.N., Jin, G.W., Chellappan, D.K., Chellian, J., and Kunnath, A.P., 2020. Bioprospecting Cultivated Tropical Green Algae, *Caulerpa* racemosa (Forsskal) J. Agardh: A Perspective on Nutritional Properties, Antioxidative Capacity and Anti-Diabetic Potential. *Foods*. Vol. 9. pp. 1-20.

Butt, S.S., Badshah, Y., Shabbir, M. dan Rafiq, M., 2020. Molecular docking using chimera and autodock vina software for nonbioinformaticians. *JMIR Bioinformatics and Biotechnology*, 1(1), 1-25.

Dayarathne, L.A., Ranaweera, S.S., Natraj, P., Rajan, P., Lee, Y.J. and Han, C.H., 2021. The effects of naringenin and naringin on the glucose uptake and AMPK phosphorylation in high glucose treated HepG2 cells. *Journal of Veterinary Science*, 22(6).

Dhorajiwala, T.M., Halder, S.T., dan Samant, L., 2019. Comparative *in silico* molecular docking analysis of l-threonine-3-dehydrogenase, a protein target against african trypanosomiasis using selected phytochemicals. *Journal of Applied Biotechnology Reports*, 6(3), 101- 108.

Endriyanto, N.C., *et al*., 2022. *In silico* Study of Srikaya Leaf Compounds (*Annona squamosa* L.) Against Protein Dihydrofolate Reductase in Mycobacterium tuberculosis. Pharmacon: *Jurnal Farmasi Indonesia*. Vol. 19. No. 1.

Faulkner, D.J. 1992. *Marine Natural Products*. Natural Product Reports, 9(4), 323-364.

Faulkner, D.J. 1995. *Marine Natural Products*. Natural Product Reports, 12(3), 223-269.

Faulkner, D.J. 2000. Highlights of Marine Natural Products Chemistry (1972–1999). *Natural product reports*, 17(1), 1-6.

ni, A., Del Frate, G., Martinelli, A., Macchia, M., Minutolo, F., & rdi, T., 2015. Development and validation of a docking-based screening platform for the identification of new lactate genase inhibitors. *Molecules*, 20(5), 8772–8790. oi.org/10.3390/molecules20058772.

z, A., D'Ambrosio, dan Pietra, F. Chim. *Acta*;1992.

Hamid, N., Razak, R., dan Najib, A., 2021. *Virtual Screening Pada Senyawa Kimia Tumbuhan Terap (Artocarpus elasticus) Terhadapprotein target Alpha Estrogen*. Pekalongan: Penerbit NEM.

Hasan, R., Herowati, R., and Widodo, G.P., 2022. *in silico* Analysis of Antidiabetic Activity And Admet Prediction Of Potential Compounds From *Luffa acutangula*. *Proceedings of The International Conference on Health Technology (ICoHT)*. Vol. 1.

Hosfield, D.J *et al*., 2005. Conformational Flexibility in Crystal Structures of Human 11β-Hydroxysteroid Dehydrogenase Type I Provide Insights into Glucocorticoid Interconversion and Enzyme Regulation. *The Journal Of Biological Chemistry*. Vol. 280, No. 6.

Hurren, K.M. and Dunham, M.W., 2021. Are Thiazolidinediones a Preferred Drug Treatment for Type 2 Diabetes?. *Expert Opinion on Pharmacotherapy*, 22(2), pp.131-133.

Khaerunnisa, S., Suhartati., dan Awaluddin, R., 2020. *Penelitian in silico untuk pemula*. Surabaya: Airlangga University Press.

Krishnan, N *et al*., 2015. PTP1B inhibition suggests a therapeutic strategy for Rett syndrome. *The Journal of Clinical Investigation*. Vol. 125. No. 8.

Liu, Z., Singh, S.B., Zheng, Y., Lindblom, P., Tice, C., Dong, C., Zhuang, L., Zhao, Y., Kruk, B.A., Lala, D., Claremon, D.A., McGeehan, G.M., Gregg, R.D., and Cain, R., 2019. Discovery of Potent Inhibitors of 11β-Hydroxysteroid Dehydrogenase Type 1 Using a Novel Growth-Based Protocol of *in silico* Screening and Optimization in CONTOUR. *Journal Chemical Information and Modeling*. Vol. 59.

Luo, J., Zhang, R., Wang, X., Hou, Z., Guo, S., & Jiang, B., 2020. Binding properties of marine bromophenols with human protein tyrosine phosphatase 1B: Molecular docking, surface plasmon resonance and cellular insulin resistance study. *International Journal of Biological Macromolecules*. Vol. 163.

Matsuzaka, Y. and Yashiro, R., 2022. Molecular Docking and Intracellular Translocation of Extracellular Vesicles for Efficient Drug Delivery. *International Journal of Molecular Sciences*, 23(21), p.12971.

t al., 2022. In-Silico Molecular Interactions Among The ary Metabolites of *Caulerpa* spp. and Colorectal Cancer *Frontiers in Chemistry*.

-wilby, M. 2008. *Molecular In silico*. 443, pp. 365– 382.

Pandelaki, K., and Sedli, B. P., 2021. Gaya Hidup sebagai isiko Diabetes Melitus Tipe 2. *E-CliniC*. Vol. 9 No. 2. 328.

Musfiroh, I., Azura, A.R., and Rahayu, D., 2020. Prediction of Asiatic Acid Derivatives Affinity Against SARS-CoV-2. Main Protease Using Molecular Docking. *Pharmaceutical Sciences and Research*. Vol. 7., No. 4.

Rao, M.M., and Hariprasad, T.P.N., 2021. *In silico* analysis of a potential antidiabetic phytochemical erythrin against therapeutic targets of diabetes. *In silico Pharmacology*. Vol. 9. No. 5.

Rendi, I.P., Maranata, J., Chaerunisa, H., Nugraheni, N. and Alfathonah, S.S., 2021. Molecular docking of compounds in moringa oleifera lam with dipeptidyl peptidase-4 receptors as antidiabetic candidates. *Jurnal Farmasi dan Ilmu Kefarmasian Indonesia*, 8(3), 242-249.

Rengasamy, K.R.R., Mahomoodally, M.F., Aumeeruddy, M.Z., Zengin, G., Xiao, j., and Kim, D.H., 2019. Bioactive Compounds in Seaweeds: An Overview of Their Biological Properties and Safety. *Food and Chemical Toxicology*.

Rochfort, S.J., Watson, R. dan Capon, R.J., 1996. Dictyosphaerin: A Novel Bicyclic Lipid From a Southern Australian Marine Green Algae, Dictyosphaeria sericea. *Journal of Natural Products*, 59(12), 1154-1156.

Rollando, R., Chandra, M.D., Aftoni, M.H., and Swastika, W., 2024. Molecular Docking and Molecular Dynamic Studies of Secondary Metabolites from *Momordica charantia* as Natural Antidiabetic. *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)*. Vol. 10., No.1.

Rosenstock J., Banarer S., Fonseca V.A., Inzucchi S.E., Sun W., Yao W., Hollis G., Flores R., Levy R., Williams W.V., Seckl J.R., Huber R., 2010. INCB13739-202 Principal Investigators. The 11-beta-hydroxysteroid dehydrogenase type 1 inhibitor INCB13739 improves hyperglycemia in patients with type 2 diabetes inadequately controlled by metformin monotherapy. *Diabetes Care*; 33(7):1516-22.

Rushdi, M.I., Imam, A.M., Rahman, A., Attia, E.Z., Abdelraheem, W.M., Saber, H., Madkour, H.A., Amin, E., Hassan, H.M., and Abdelmoshsen, U.R., 2020. A Review on the Diversity, Chemical, and Pharmacologycal Potential of the Green Algae Genus *Caulerpa*. *South African Journal of Botany*. Vol 123. Pp 226-241.

2023. Green Seaweed *Caulerpa* racemosa - Chemical ents, Cytotoxicity in Breast Cancer Cells and Molecular Simulation. *Journal of Agriculture and Food Research*. Vol.

i N., Kusumaningtyas E., Priyatama D., Santoso B., 2016. Molekular Potensi Anti Diabetes Melitus Tipe 2 Turunan

Zerumbon Sebagai Inhibitor Aldosa Reduktase Dengan Autodock-Vina. *Chim Nat Acta*; 4(1):16. Doi:10.24198/can.v4.n1.10443.

Scheuer, P.J. dan Higa, T., 1987. Bioorganic marine chemistry. Springer-Verlag.

Sugiarto., Diding H.P., Guntur, H., Marsetio, D., and Tjokroprawiro, A., 2009. *Jurnal Kedokteran Yarsi*. Vol. 17., No. 3.

Tarry-Adkins, J.L., Grant, I.D., Ozanne, S.E., Reynolds, R.M. and Aiken, C.E., 2021. Efficacy and side effect profile of different formulations of metformin: a systematic review and meta-analysis. *Diabetes Therapy*, 12(7), pp.1901-1914.

The Lancet., 2023. Global, regional, and national burden of diabetes from 1990 to 2021, with projections of prevalence to 2050: a systematic analysis for the Global Burden of Disease Study 2021. *The Lancet*. Vol. 402.

Tringali, C. 1997. Bioactive Metabolites from Marine Algae: Recent Results. Curr. *Org. Chem*, 1(4), 375-394.

Vo, T.H.N., Tran, N., Nguyen, D., and Le, L., 2016. An *in silico* Study on Antidiabetic Activity of Bioactive Compounds in Euphorbia thymifolia Linn. SpringerPlus. DOI 10.1186/s40064-016-2631-5.

Weng, Yi-Zhong., Chang, D.T.H., and Lin, C.W., 2011. A study on the flexibility of enzyme active sites. *BMC Bioinformatics*. Vol. 11. No. 1.

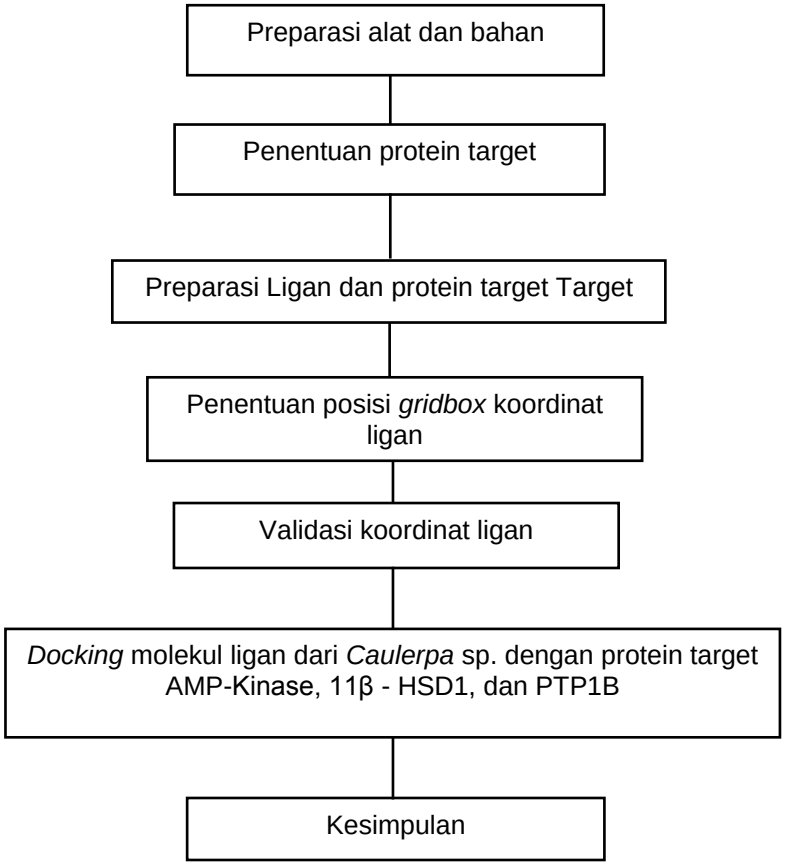
Winardi, D.O., *et al*., 2023. *In silico* and In Vitro Studies on Compounds in Turmeric (*Curcuma domestica*) as Anti-inflammatory for Cyclooxygenase-2 (COX-2. *Indonesian Journal of Pharmaceutical Science and Technology*. Vol.1., No.1.

Yang, P., Liu, D.Q., Liang, T.J., Li, J., Zhang, H.Y., Liu, A.H., Guo, Y.W. and Mao, S.C., 2015. Bioactive Constituents from The Green Alga *Caulerpa* racemosa. *Bioorganic & Medicinal Chemistry*. Vol. 23. No. 1. 38-45.

Yogi, W.K., and Komalasari, H., 2022. Potensi Alga Hijau (*Caulerpa* racemosa) Sebagai Sumber Antioksidan Alami. *Jurnal Teknologi dan Mutu Pangan*. Vol. 1., No. 1.

LAMPIRAN

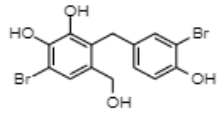
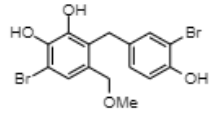
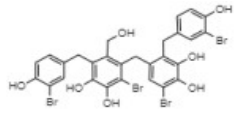
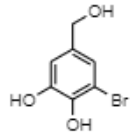
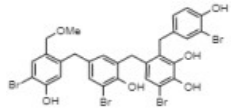
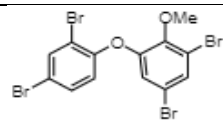
Lampiran 1.Skema Kerja

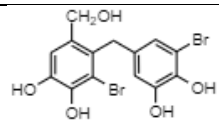


Lampiran 2. Senyawa Kandungan *Caulerpa* sp.

2.1 Golongan Fenolik

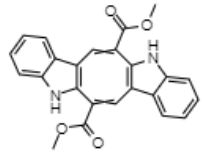
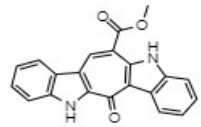
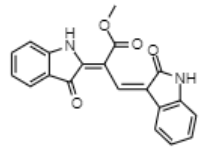
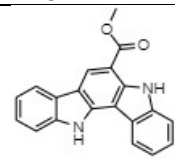
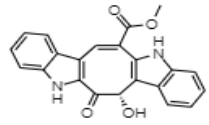
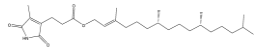
Tabel 11. Struktur 2 dimensi senyawa kandungan *Caulerpa* sp. golongan fenolik

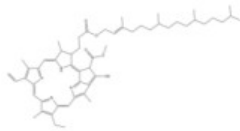
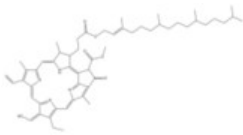
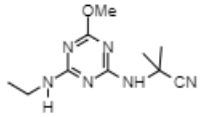
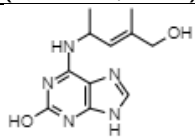
No.	Senyawa	Golongan Senyawa	Struktur	SMILES
1.	Senyawa 1	Fenolik	 (Scheuer dan Higa, 1987)	OCC1=CC(Br)=C(O)C(O)=C1CC1=CC=C(O)C(Br)=C1
2.	Senyawa 2	Fenolik	 (Tringali, 1997)	BrC(C=C1COC)=C(C(O)=C1CC2=CC=C(C(Br)=C2)O)O
3.	Senyawa 3	Fenolik	 (Tringali, 1997)	OC1=CC=C(CC2=C(O)C(O)=C(Br)C(CC3=CC(Br)=C(O)C(O)=C3CC4=CC=C(O)C(Br)=C4)=C2CO)C=C1Br
4.	Senyawa 4	Fenolik	 (Tringali, 1997)	OC1=CC(CO)=CC(Br)=C1O
5.	Senyawa 5	Fenolik	 (Tringali, 1997)	BrC1=CC(COC)=C(CC2=CC(Br)=C(O)C(CC3=CC(Br)=C(O)C(O)=C3CC4=CC=C(O)C(Br)=C4)=C2)C=C1O
		Fenolik	 (Tringali, 1997)	BrC1=C(OC)C(OC2=C(Br)C=C(Br)C=C2)=CC(Br)=C1

7.	Senyawa 7	Fenolik	 (Scheuer dan Higa, 1987)	OC1=CC(CO)=C(CC2=CC(O)=C(O)C(Br)=C2)C(Br)=C1O

2.2 Golongan Alkaloid

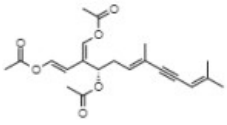
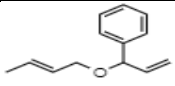
Tabel 12. Struktur 2 dimensi senyawa kandungan *Caulerpa* sp. golongan alkaloid

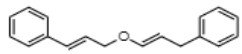
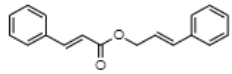
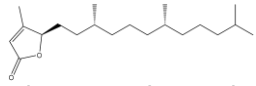
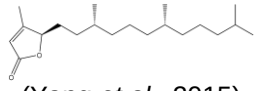
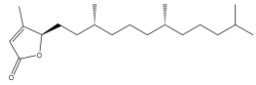
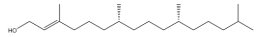
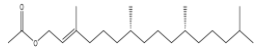
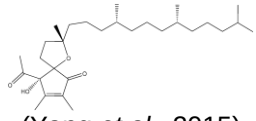
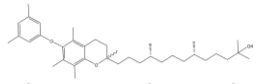
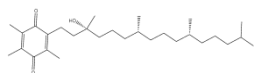
No.	Senyawa	Golongan Senyawa	Struktur	SMILES
1.	Caulerpin	Alkaloid	 (Yang *et al*. 2015)	COC(=O)C1=CC2=C(C(=CC3=C1NC4=CC=CC=C43)C(=O)OC)NC5=CC=CC=C52
2.	Caulersin	Alkaloid	 (Yang *et al*. 2015)	O=C1C2=C(C3=CC=CC=C3N2[H])C=C(C(OC)=O)C4=C1C5=CC=CC=C5N4[H]
3.	Racemosin A	Alkaloid	 (Yang *et al*. 2015)	O=C(C1=CC=CC=C1N/2)C2=C(C(OC)=O)/C=C3C4=C(NC/3=O)C=CC=C4
4.	Racemosin B	Alkaloid	 (Yang *et al*. 2015)	O=C(OC)C1=CC2=C(C3=C1NC4=C3C=CC=C4)NC5=CC=CC=C52
5.	Racemosin C	Alkaloid	 (Yang *et al*. 2015)	O=C1C2=C(C3=CC=CC=C3N2)/C=C(C(OC)=O)\C4=C(C(C=CC=C5)=C5N4)[C@@H]1O
		Alkaloid	 (Scheuer dan Higa, 1987)	CCC/CC=C/COC(CCC1=CCC(NC1=O)=O)=O

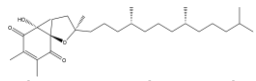
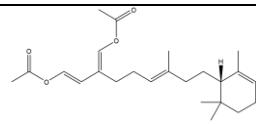
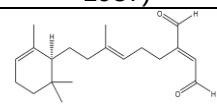
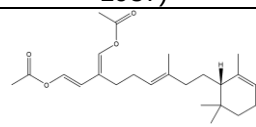
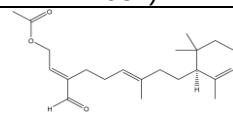
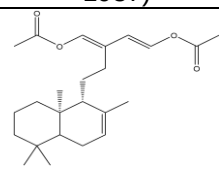
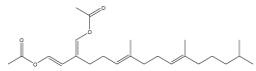
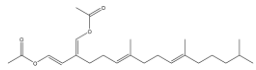
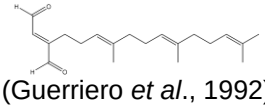
7.	Senyawa 9	Alkaloid	 (Yang *et al*. 2015)	CCC1=C(C2=NC1=CC3=C(C4=C(C(C(=C5C(C(C(=CC6=NC(=C2)C(=C6C)C=C)N5)C)CCC(=O)OCC=CCCCCCCCCCCCCCCCCC)C4=N3)C(=O)OC)O)C)C
8.	Senyawa 10	Alkaloid	 (Scheuer dan Higa, 1987)	CCC1=C2C=C3C(=C4C(=O)C(C(=C5C(C(C(=CC6=NC(=CC(=N2)C1=CO)C(=C6C)C=C)N5)C)CCC(=O)OCC=CCCCCCCCCCCCCCCCCC)C4=N3)C(=O)OC)C
9.	Senyawa 11	Alkaloid	 (Faulkner, 2000)	CCN(C1=NC(NCCCC#N)=NC(OC)=N1)[H]
10.	Senyawa 12	Alkaloid	 (Faulkner, 1995)	CC(/C=CC/CO)NC1=NC(O)=NC2=C1N=CN2

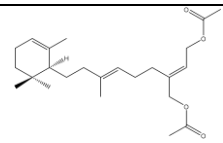
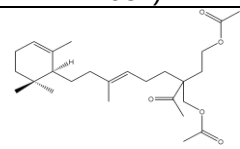
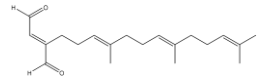
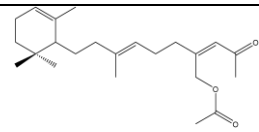
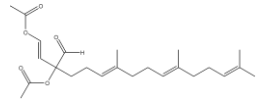
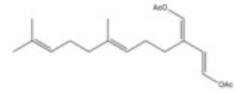
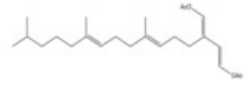
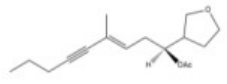
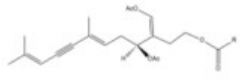
2.3 Golongan Terpenoid

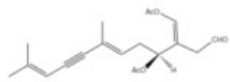
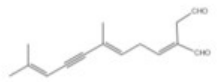
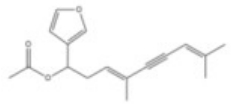
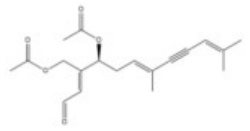
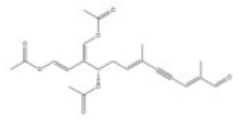
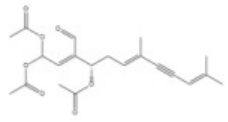
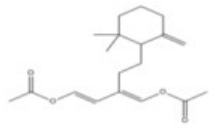
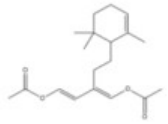
Tabel 13. Struktur 2 dimensi senyawa kandungan *Caulerpa* sp. golongan terpenoid

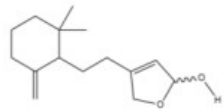
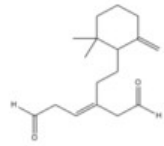
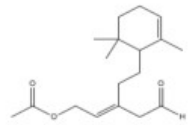
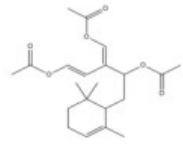
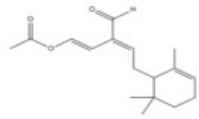
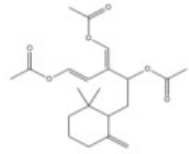
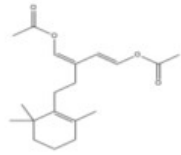
No.	Senyawa	Golongan Senyawa	Struktur	SMILES
	n	Terpenoid	 (Yang *et al.* 2015)	CC(=CC#C/C(=C/C[C@@H](/C(=C\OC(=O)C)/C=C/OC(=O)C)OC(=O)C)/C)C
	3	Terpenoid	 (Faulkner, 1992)	C\C=C\COC(C=C)C1=CC=CC=C1

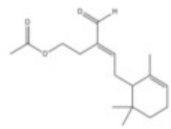
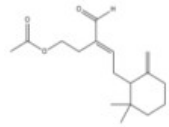
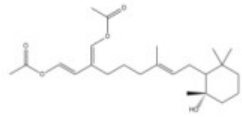
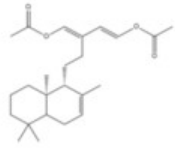
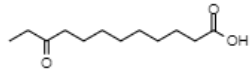
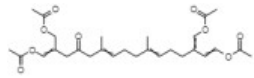
3.	Senyawa 14	Terpenoid	 (Faulkner, 1992)	C(O\C=C\CC1=CC=CC=C1)\C=C\C1=CC=CC=C1
4.	Senyawa 15	Terpenoid	 (Faulkner, 1992)	O=C(OC\C=C\C1=CC=CC=C1)\C=C\C1=CC=CC=C1
5.	Senyawa 16	Terpenoid	 (Yang *et al.,* 2015)	O=C1C=CC[C@@H](CC[C@H]CCCC[C@H]CCCCCCC)O1
6.	Senyawa 17	Terpenoid	 (Yang *et al.,* 2015)	O=C1C=CC[C@H](CC[C@H]CCCC[C@H]CCCCCCC)O1
7.	Senyawa 18	Terpenoid	 (Yang *et al.,* 2015)	C[C@H](CCC[C@H]CCCCCCC)CCCC1=CC(OC1O)=O
8.	Senyawa 19	Terpenoid	 (Yang *et al.,* 2015)	OC/C=CC/CCC[C@H]CCCC[C@H]CCCCCCC
9.	Senyawa 20	Terpenoid	 (Yang *et al.,* 2015)	CC(OC/C=CC/CCC[C@H]CCCC[C@H]CCCCCCC)=O
10.	Senyawa 21	Terpenoid	 (Yang *et al.,* 2015)	C[C@H](CCC[C@H]CCCCCCC)CCC[C@@]1CCCC2([C@](O)(CC=O)CC=CCC2=O)O1
11.	Senyawa 22	Terpenoid	 (Yang *et al.,* 2015)	CC1=CC(OC2=CCCC=C(OC(CCC[C@H]CCC[C@H]CCCCCCC)CCC3)C3=C2C)=CCC=C1
	3	Terpenoid	 (Yang *et al.,* 2015)	CC1=CCC(CC=C(CC[C@]C(O)CCC[C@H]CCCC[C@H]CCCCCCC)C1=O)=O

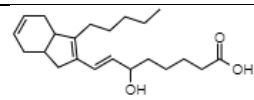
13.	Senyawa 24	Terpenoid	 (Yang *et al.,* 2015)	C[C@H](CCC[C@H]CCCCCC)CCC[C@]1CCC([C@]2(O)C(CC=CCC3=O)=O)[C@@]23O1
14.	Senyawa 25	Terpenoid	 (Scheuer dan Higa, 1987)	[C@@H]1(CCCC=CCC\C(=C/OCC=O)C=COCC=O)C(=CCCC1CC)C
15.	Senyawa 26	Terpenoid	 (Scheuer dan Higa, 1987)	C([H])(=O)C=C(CCC=CCCC[C@@H]1C(=CCCC1CC)C)C([H])=O
16.	Senyawa 27	Terpenoid	 (Scheuer dan Higa, 1987)	[C@@H]1(CCCC=CCCC(COCC=O)=CCOCC=O)C(=CCCC1CC)C
17.	Senyawa 28	Terpenoid	 (Scheuer dan Higa, 1987)	C([H])(=O)C(CCC=CCCC[C@@H]1C(=CCCC1CC)C)=CCOCC=O
18.	Senyawa 29	Terpenoid	 (Scheuer dan Higa, 1987)	CC(=O)O\C=C\C(\CC[C@@H]1CC=CCC2CCCCCC[C@@]12C)=C\OCC=O
19.	Senyawa 30	Terpenoid	 (Guerriero *et al*., 1992)	CCCCCC\CC=C\CC\CC=C\CC\C(=C/OCC=O)\C=C\OCC=O
	1	Terpenoid	 (Guerriero *et al*., 1992)	CCC=CCCCC=CCCCC=CCC\C(=C/OCC=O)C=COCC=O
	2	Terpenoid	 (Guerriero *et al*., 1992)	C([H])(=O)C=C(CCC=CCCCC=CCCCC=CCC)C([H])=O

22.	Senyawa 33	Terpenoid	 (Scheuer dan Higa, 1987)	[C@@H]1(CCCC=CCCC(COCC=O)=CCOCC=O)C(=CCCC1CC)C
23.	Senyawa 34	Terpenoid	 (Scheuer dan Higa, 1987)	C([H])(=O)C(CCC=CCCC[C@@H]1C(=CCCC1CC)C)(COCC=O)C=COCC=O
24.	Senyawa 35	Terpenoid	 (Guerriero *et al*., 1992)	C([H])(=O)C=C(CCC=CCCCC=CCCCC=CCC)COCC=O
25.	Senyawa 36	Terpenoid	 (Scheuer dan Higa, 1987)	C([H])(C=C(COCC=O)CCC=C(CC[C@@H]1C(=CCCC1CC)C)C)=O
26.	Senyawa 37	Terpenoid	 (Guerriero *et al*., 1992)	C([H])(=O)C(CCC=CCCCC=CCCCC=CCC)(OCC=O)C=COCC=O
27.	Senyawa 38	Terpenoid	 (Scheuer dan Higa, 1987)	CCC=CCCCC=CCC\C(C=COCC=O)=C/OCC=O
28.	Senyawa 39	Terpenoid	 (Scheuer dan Higa, 1987)	C/C(CCCCCC)=C\CC/CC=C/CCC(/C=C/OCC=O)=C\OCC=O
29.	Senyawa 40	Terpenoid	 (Guerriero *et al*., 1992)	[C@H](OCC=O)(C1CCOC1)CC=C(C#CCCC)C
	1	Terpenoid	 (Guerriero *et al*., 1992)	CC(OCC\C([C@@H](CC=C(C#CC=CCC)C)OCC=O)=C\OCC=O)=O

31.	Senyawa 42	Terpenoid	 (Guerriero *et al*., 1992)	[H][C@](C/C=C(C#C/C=CC\C)\C)(OCC=O)/C(CC([H])=O)=C\OCC=O
32.	Senyawa 43	Terpenoid	 (Guerriero *et al*., 1992)	CC(C#CC=CCC)=CCC=C(CC([H])=O)C([H])=O
33.	Senyawa 44	Terpenoid	 (Guerriero *et al*., 1992)	CC(=CC#CC(=CCC(C1=COC=C1)OC(=O)C)C)C
34.	Senyawa 45	Terpenoid	 (Guerriero *et al*., 1992)	CC(=CC#CC(=CC[C@@H](C(=CC=O)COC(=O)C)OC(=O)C)C)C
35.	Senyawa 46	Terpenoid	 (Guerriero *et al*., 1992)	C/C(=C\C[C@@H](/C(=C\OC(=O)C)/C=C/OC(=O)C)OC(=O)C)/C#C/C=C(\C)/C=O
36.	Senyawa 47	Terpenoid	 (Guerriero *et al*., 1992)	CC(=CC#CC(=CC[C@@H](C(=CC(OC(=O)C)OC(=O)C)C=O)OC(=O)C)C)C
37.	Senyawa 48	Terpenoid	 (Scheuer dan Higa, 1987)	C1C(C(C(CC1)CC)CC\C(=C/OCC=O)C=COCC=O)=C
	9	Terpenoid	 (Scheuer dan Higa, 1987)	C1=C(C(C(CC1)CC)CC\C(=C/OCC=O)C=COCC=O)C

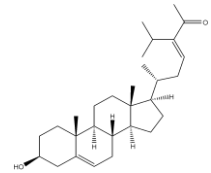
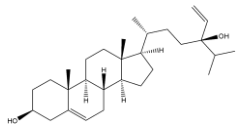
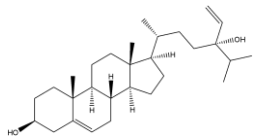
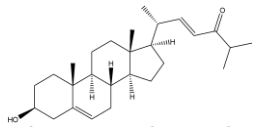
39.	Senyawa 50	Terpenoid	 (Scheuer dan Higa, 1987)	CC1(C)C(CCC2=CC(O)OC2)C(CCC1)=C
40.	Senyawa 51	Terpenoid	 (Scheuer dan Higa, 1987)	C1C(C(C(CC1)(C)C)CCC(CC(=O)[H])=CCC(=O)[H])=C
41.	Senyawa 52	Terpenoid	 (Scheuer dan Higa, 1987)	C1=C(C(C(CC1)CC)CCC(CC(=O)[H])=CCOCC=O)C
42.	Senyawa 53	Terpenoid	 (Scheuer dan Higa, 1987)	C1=C(C(C(CC1)CC)CC(\C(=C\OCC=O)C=COCC=O)OCC=O)C
43.	Senyawa 54	Terpenoid	 (Scheuer dan Higa, 1987)	[H]C(=O)\C(=C\CC1CC=CCCC1CC)\C=C\OCC=O
44.	Senyawa 55	Terpenoid	 (Scheuer dan Higa, 1987)	C1CCC(C(C1=C)CC(\C(=C\OCC=O)C=COCC=O)OCC=O)CC
	6	Terpenoid	 (Scheuer dan Higa, 1987)	C1CCC(C(=C1C)CC\C(=C\OCC=O)C=COCC=O)CC

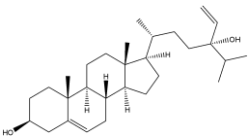
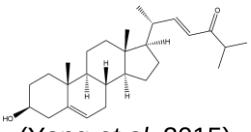
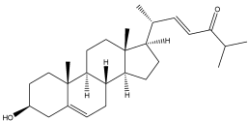
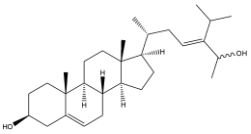
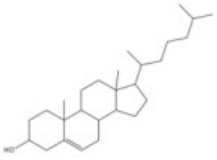
46.	Senyawa 57	Terpenoid	 (Scheuer dan Higa, 1987)	[H]C(=O)C(\CCOCC=O)=C\CC1CC=CCCC1CC
47.	Senyawa 58	Terpenoid	 (Scheuer dan Higa, 1987)	[H]C(=O)C(\CCOCC=O)=C\CC1C(=C)CCCC1CC
48.	Senyawa 59	Terpenoid	 (Scheuer dan Higa, 1987)	CC(=O)OC=C\C(CCCCC=CCC1CCCCCC[C@]1CO)=C\OCC=O
49.	Senyawa 60	Terpenoid	 (Scheuer dan Higa, 1987)	CC(=O)O\C=C\C(\CC[C@@H]1CC=CCC2CCCCCC[C@@]12C)=C\OCC=O
50.	Senyawa 61	Terpenoid	 (Scheuer dan Higa, 1987)	CCC=CCCCC=CCCCC=CCCC=CCCCC=CCCC[C@H](O)CC=C
51.	Senyawa 62	Terpenoid	 (Scheuer dan Higa, 1987)	CC(=CCCC(=CCCC(=CCCC1C(O1)CCCC=CCCCC=CCC)C)C)C
52.	Senyawa 63	Terpenoid	 (Scheuer dan Higa, 1987)	CCC(CCCCCCCCC(O)=O)=O
	4	Terpenoid		CC(=CCCC(=COC(=O)C)C=COC(=O)C)CCC=CCCC(=O)CC(=COC(=O)C)COC(=O)C

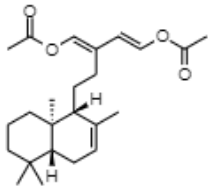
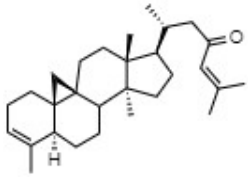
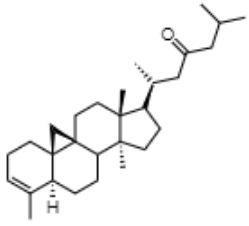
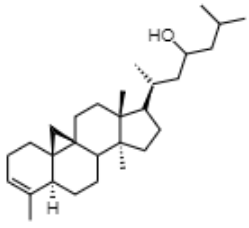
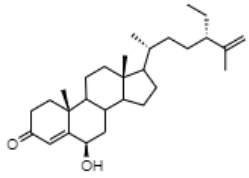
54.	Senyawa 65	Terpenoid	 (Rochfort *et al*., 1996)	CCCCCC1=C(/C=C/C(O)CCCCC(O)=O)CC2C1CC=CC2

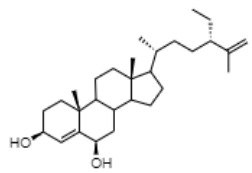
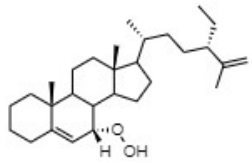
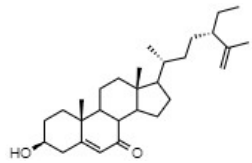
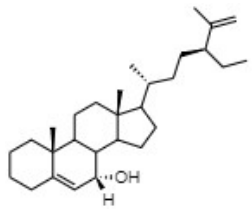
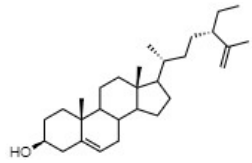
2.4 Golongan Steroid

Tabel 14. Struktur 2 dimensi senyawa kandungan *Caulerpa* sp. golongan steroid

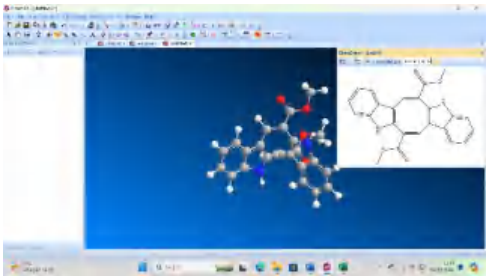
No.	Senyawa	Golongan Senyawa	Struktur	SMILES
1.	Senyawa 66	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CC\C=C(/CCC)CC=O
2.	Senyawa 67	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CCC[C@](O)(C=C)CCC
3.	Senyawa 68	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CCC[C@@](O)(C=C)CCC
	9	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]C\C=C\C(=O)CCC

5.	Senyawa 70	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CCC\C(=C/C)CCC
6.	Senyawa 71	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CCC[C@@]1(O[C@H]1C)CCC
7.	Senyawa 72	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CCC[C@]1(O[C@@H]1C)CCC
8.	Senyawa 73	Steroid	 (Yang *et al*. 2015)	[H][C@@]1(CC[C@@]2([H])[C@]3([H])CC=C4C[C@@H](O)CC[C@]4C[C@@]3([H])CC[C@]12C)[C@H]CC\C=C(/CCC)CCO
9.	Senyawa 74	Steroid	 (Rochfort *et al*., 1996)	CCCCCCCCC1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C

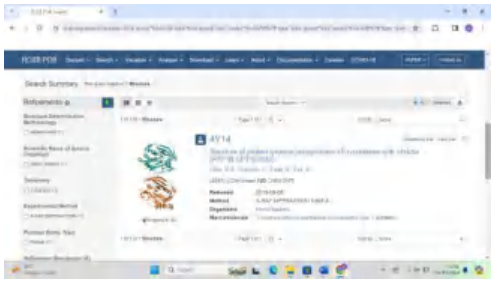
10.	Senyawa 75	Steroid	 (Scheuer dan Higa, 1987)	[H]C1(CC\C(=C/OCC=O)\C=C\OCC=O)CC=CC[C@]2([H])CCCCCC[C@@]12C
11.	Senyawa 76	Steroid	 (Scheuer dan Higa, 1987)	C[C@@]12[C@](CC[C@@H]2[C@@H](CC(/C=CC/C)=O)C)CC3CC[C@@]4([H])CC=CCC[C@]4(C5)[C@]35CC1
12.	Senyawa 77	Steroid	 (Scheuer dan Higa, 1987)	C[C@]12[C@]C(C3CC[C@]4(CC=CCC[C@@]45C[C@]53CC2)[H])CC[C@H]1CCCC(CCCC)=O
13.	Senyawa 78	Steroid	 (Scheuer dan Higa, 1987)	C[C@]12[C@]C(C3CC[C@]4(CC=CCC[C@@]45C[C@]53CC2)[H])CC[C@H]1CCCC(O)CCCC
	9	Steroid	 (Rochfort *et al*., 1996)	O=C1CC[C@@]2CC([C@H](O)CC3C2CC[C@@]4CC3CCC4[C@H]CCC[C@H](CC)CC=C)=C1

15.	Senyawa 80	Steroid	 (Rochfort *et al*., 1996)	CC[C@@H](CC[C@@H]CC1CCC2C3C[C@@H](O)C4=C[C@@H](O)CC[C@]4CC3CC[C@]12C)CC=C
16.	Senyawa 81	Steroid	 (Rochfort *et al*., 1996)	CC[C@H](CC=C)CC[C@H](C1CCC2C3[C@]([H])(O)C=C4CCCC[C@@]4(C3CC[C@]12C)C)C
17.	Senyawa 82	Steroid	 (Rochfort *et al*., 1996)	C[C@H](CC[C@H](CC)CC=C)C1CCC2C3C(C=C4C[C@@H](O)CC[C@@]4(C3CC[C@@]21C)C)=O
18.	Senyawa 83	Steroid	 (Rochfort *et al*., 1996)	C[C@@H](C1CCC2C3[C@]([H])(O)C=C4CCCC[C@]4CC3CC[C@@]21C)CC[C@@H](CC=C)CC
19.	Senyawa 84	Steroid	 (Rochfort *et al*., 1996)	C[C@H](CC[C@H](CC)CC=C)C1CCC2C3CC=C4C[C@@H](O)CC[C@@]4(C3CC[C@@]21C)C

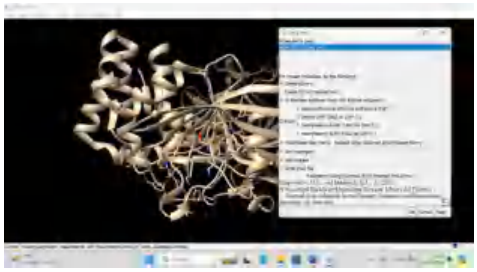
Lampiran 3. Dokumentasi Penelitian



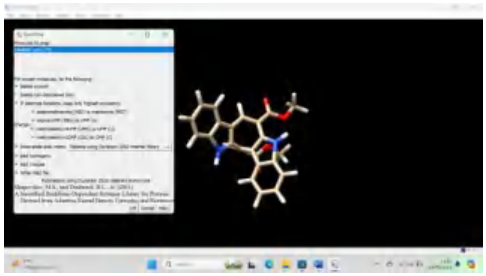
Gambar 15. Proses mendapatkan smiles



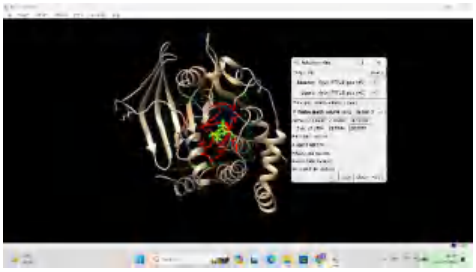
Gambar 16. Proses pemilihan ID PDBprotein target yang akan digunakan



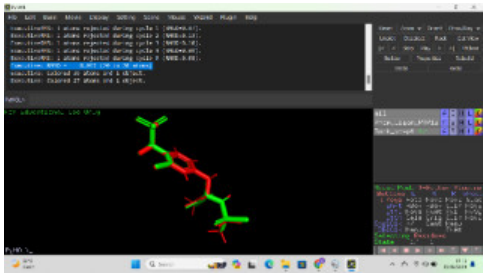
Gambar 17. Proses preparasi enzim dan ligan alami



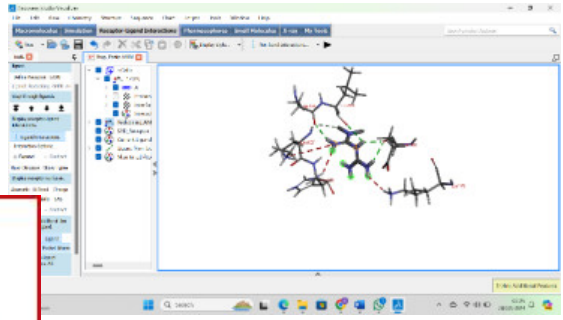
Gambar 18. Proses preparasi senyawa pada *Caulerpa* sp.



Gambar 19. Proses Penentuan *Gridbox* pada masing-masing enzim



Gambar 20. Proses Memperoleh Hasil RMSD pada Ligan Alami



ses Visualisasi menggunakan Discovery Studio Visualizer