

DAFTAR PUSTAKA

- Adelya, L., Dewi, P. C., Auw, Z. C., Winengku, R. T. P., Mase, M., Setyaningsih, D., & Riswanto, F. D. O. (2022). Potensi Herba Bandotan (*Ageratum conyzoides* L.) sebagai Agen Antikanker Payudara. *Cendekia Journal of Pharmacy*, 6(1), 1–12. <https://doi.org/10.31596/cjp.v6i1.153>
- Amin, A., Naveed, M., Sarwar, A., Rasheed, S., Saleem, H. G. M., Latif, Z., & Bechthold, A. (2022). In vitro and in silico Studies Reveal *Bacillus cereus* AA-18 as a Potential Candidate for Bioremediation of Mercury-Contaminated Wastewater. *Frontiers in Microbiology*, 13(June), 1–13. <https://doi.org/10.3389/fmicb.2022.847806>
- Arazu, V. A., Nelson, C., Henrietta, U. O., Akinwonmi, A., Ochebo, A. S., & Samuel, C. (2022). Inhibitory Effect of Gedunin Analogue against the *Plasmodium falciparum* Dihydrofolate Reductase. *Asian Journal of Research in Biochemistry*, 11(1), 1–10. <https://doi.org/10.9734/ajrb/2022/v11i130234>
- Aziz, A., Andrianto, D., & Safithri, M. (2022). Penambatan Molekuler Senyawa Bioaktif Daun Wungu (*Graptophyllum Pictum* (L) Griff) sebagai Inhibitor Tirosinase. *Indonesian Journal of Pharmaceutical Science and Technology*, 9(2), 94. <https://doi.org/10.24198/ijpst.v9i2.36219>
- Cahyawati, P. N. (2018). Imunoterapi pada Kanker Payudara. *WICAKSANA, Jurnal Lingkungan & Pembangunan*, 2(1), 52–55.
- Cao, C., Wang, L., Chen, X., Zou, S., Wang, G., & Xu, S. (2015). Amino Acids in Nine Ligand-Prefer Ramachandran Regions. *BioMed Research International*, 2015. <https://doi.org/10.1155/2015/757495>
- Chen, X., Li, H., Tian, L., Li, Q., Luo, J., & Zhang, Y. (2020). Analysis of the Physicochemical Properties of Acaricides Based on Lipinski's Rule of Five. *Journal of Computational Biology*, 27(9), 1397–1406. <https://doi.org/10.1089/cmb.2019.0323>
- Chow, E., Rendleman, C. A., Bowers, K. J., Dror, R. O., H, D., Gullingsrud, J., Sacerdoti, F. D., & Shaw, D. E. (2008). Desmond Performance on a Cluster of Multicore Processors. *Simulation, July*, 1–14.
- DasGupta, D., Kaushik, R., & Jayaram, B. (2015). From Ramachandran Maps to Tertiary Structures of Proteins. *Journal of Physical Chemistry B*, 119(34), 11136–11145. <https://doi.org/10.1021/acs.jpcc.5b02999>
- Dash, R., Ali, M. C., Dash, N., Azad, M. A. K., Zahid Hosen, S. M., Hannan, M. A., & Moon, I. S. (2019). Structural and dynamic characterizations highlight the deleterious role of SULT1A1 R213H polymorphism in substrate binding. *International Journal of Molecular Sciences*, 20(24). <https://doi.org/10.3390/ijms20246256>
- Dwi, D. K., Sasongkowati, R., & Haryanto, E. (2020). Studi in Silico Sifat Farmakokinetik, Toksisitas, Dan Aktivitas Imunomodulator Brazilein Kayu Secang Terhadap Enzim 3-Chymotrypsin-Like Cysteine Protease Coronavirus. *Journal of Indonesian Medical Laboratory and Science (JoImedLabs)*, 1(1), 76–85. <https://doi.org/10.53699/joimedlabs.v1i1.14>
- El-Hachem, N., Haibe-Kains, B., Khalil, A., Kobeissy, F. H., & Nemer, G. (2017). AutoDock and AutoDockTools for protein-ligand docking: Beta-site amyloid precursor protein cleaving enzyme 1(BACE1) as a case study. *Methods in*

Molecular Biology, 1598, 391–403. https://doi.org/10.1007/978-1-4939-6952-4_20

- Febri, F. A., Chilfi, T., Salamah, A. F., & Wilipangga, A. (2023). Analisis Farmakokinetik Dan Toksisitas Pada Kandungan Fenolik Ekstrak Daun Salam (*Syzygium polyanthum*) Menggunakan In Silico pkCMS Dan Prottox II. *Jurnal Bina Cipta Husada*, 19(1), 108–117.
- Hanif, A. U., Lukis, P. A., & Fadlan, A. (2020). Pengaruh Minimisasi Energi MMFF94 dengan MarvinSketch dan Open Babel PyRx pada Penambatan Molekular Turunan Oksindola Tersubstitusi. *Alchemy*, 8(2), 33–40. <https://doi.org/10.18860/al.v8i2.10481>
- Islam, M. K., Barman, A. C., & Qais, N. (2020). Anti-Cancer Constituents from Plants: Mini Review. *Dhaka University Journal of Pharmaceutical Sciences*, 19(1), 83–96. <https://doi.org/10.3329/dujps.v19i1.47823>
- Kalontong, P. K., Safithri, M., & Tarman, K. (2022). Molecular Docking of Active Compound of *Spirulina platensis* as TMPRSS2 Inhibitor to Prevent the SARS-COV-2 Infection. *Jurnal Pengolahan Hasil Perikanan Indonesia*, 25(2), 253–267. <https://doi.org/10.17844/jphpi.v25i2.40645>
- Kesuma, D., Siswandono, S., Purwanto, B. T., & Hardjono, S. (2018). Uji in silico Aktivitas Sitotoksik dan Toksisitas Senyawa Turunan N-(Benzoil)-N'-feniltiourea Sebagai Calon Obat Antikanker. *JPSCR: Journal of Pharmaceutical Science and Clinical Research*, 3(1), 1. <https://doi.org/10.20961/jpscr.v3i1.16266>
- Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J., & Bolton, E. E. (2021). PubChem in 2021: New data content and improved web interfaces. *Nucleic Acids Research*, 49(D1), D1388–D1395. <https://doi.org/10.1093/nar/gkaa971>
- Kotta, J. C., Lestari, A. B. S., Candrasari, D. S., & Hariono, M. (2020). Medicinal Effect, in Silico Bioactivity Prediction, and Pharmaceutical Formulation of *Ageratum conyzoides* L.: A Review. *Scientifica*, 2020. <https://doi.org/10.1155/2020/6420909>
- Kumar, S., Sharma, P. P., Upadhyay, C., Kempaiah, P., Rathi, B., & Poonam. (2021). Multi-targeting approach for nsp3, nsp9, nsp12 and nsp15 proteins of SARS-CoV-2 by Diosmin as illustrated by molecular docking and molecular dynamics simulation methodologies. *Methods*, 195(February 2021), 44–56. <https://doi.org/10.1016/j.ymeth.2021.02.017>
- Lailiyah, H., & Lisdiana, L. (2023). Uji Aktivitas Antibakteri Senyawa Aktif Temu Kunci (*Boesenbergia rotunda*) Terhadap *Mycobacterium tuberculosis* Secara In Silivo. *LenteraBio: Berkala Ilmiah Biologi*, 12(2), 132–149. <https://doi.org/10.26740/lenterabio.v12n2.p132-149>
- Lipinski, C. A. (2004). Lead- and drug-like compounds: The rule-of-five revolution. *Drug Discovery Today: Technologies*, 1(4), 337–341. <https://doi.org/10.1016/j.ddtec.2004.11.007>
- Lu, H.-M., Yin, D.-C., Ye, Y.-J., Luo, H.-M., Geng, L.-Q., Li, H.-S., Guo, W.-H., & Shang, P. (2009). Correlation Between Protein Sequence Similarity and X-Ray Diffraction Quality in the Protein Data Bank. *Protein & Peptide Letters*, 16(1), 50–55. <https://doi.org/10.2174/092986609787049457>
- Łukasiewicz, S., Czezelewski, M., Forma, A., Baj, J., Sitarz, R., & Stanisławek, A. (2021). Breast Cancer—Epidemiology, Risk Factors, Classification,

- Prognostic Markers, and Current Treatment Strategies— An Updated Review. *Cancers*, 13(4287), 1–30. <https://doi.org/https://doi.org/10.3390/cancers13174287>
- Mardianingrum, R., Bachtiar, K. R., Susanti, S., Aas Nuraisah, A. N., & Ruswanto, R. (2021). Studi In Silico Senyawa 1,4-Naphthalenedione-2-Ethyl-3-Hydroxy sebagai Antiinflamasi dan Antikanker Payudara. *ALCHEMY Jurnal Penelitian Kimia*, 17(1), 83. <https://doi.org/10.20961/alchemy.17.1.43979.83-95>
- Mardianingrum, R., Endah, S. R. N., Suhardiana, E., Ruswanto, R., & Siswandono, S. (2021). Docking and molecular dynamic study of isoniazid derivatives as anti-tuberculosis drug candidate. *Chemical Data Collections*, 32, 100647. <https://doi.org/10.1016/j.cdc.2021.100647>
- Mary, A. P. F., & Giri, R. S. (2016). Phytochemical Screening and Gc-Ms Analysis in Ethanolic Leaf Extracts of *Ageratum Conyzoides* (L .). *World Journal of Pharmaceutical Research*, 5(7), 1019–1029. <https://doi.org/10.20959/wjpr20167-6505>
- Melissa, & Muchtaridi, M. (2017). Senyawa aktif dan manfaat farmakologis *Ageratum conyzoides*. *Farmaka*, 15(1), 200–2012.
- Mills, K. A., Chess-Williams, R., & McDermott, C. (2019). Novel insights into the mechanism of cyclophosphamide-induced bladder toxicity: chloroacetaldehyde’s contribution to urothelial dysfunction in vitro. *Archives of Toxicology*, 93(11), 3291–3303. <https://doi.org/10.1007/s00204-019-02589-1>
- Nugraha, W., Suwartawan, W., Prayoga, A., Laksmiani, L., Putra, P., & Ani, S. (2018). Potensi Brazilein Potensi Brazilein dari Kayu Secang (*Caesalpinia sappan* L.) Sebagai Agen Depigmentasi Kulit Secara In Silico. *Jurnal Farmasi Udayana*, 7(1), 1. <https://doi.org/10.24843/jfu.2018.v07.i01.p02>
- Nursanti O. (2019). Validasi Penambatan Molekul Untuk Mendapatkan Ligan Aktif Pada Reseptor Cyclooxygenase 2. *Prosiding Seminar Informasi Kesehatan Nasional*, 411–430.
- Pinzi, L., & Rastelli, G. (2019). Metode berbasis struktur bergantung pada informasi yang diperoleh dari pengetahuan tentang struktur 3D target yang menarik, dan mereka memungkinkan database peringkat molekul sesuai dengan struktur dan komplementaritas elektronik ligan ke target tertentu. *Igms in Drug Discovery. InternatInPinzi, L., & Rastelli, G. (2019). Molecular Docking: Shifting Paradional Journal of Molecular Sciences*, 20(18). <https://doi.org/10.3390/Ijms20184331> *International Journal of Molecular Sciences*, 20(18), 1–23.
- Pollastri, M. P. (2010). Overview on the rule of five. *Current Protocols in Pharmacology*, SUPPL. 49, 1–8. <https://doi.org/10.1002/0471141755.ph0912s49>
- Puratchikody, A., Sriram, D., Umamaheswari, A., & Irfan, N. (2016). 3-D structural interactions and quantitative structural toxicity studies of tyrosine derivatives intended for safe potent inflammation treatment. *Chemistry Central Journal*, 10(1), 1–19. <https://doi.org/10.1186/s13065-016-0169-9>
- Rollando. (2017). *Pengantar Kimia Medisinal*.
- Ruswanto, Richa Mardianingrum Siswandono, Dini Kesuma, et al. (2020). Reverse Docking, Molecular Docking, Absorption, Distribution, and Toxicity Prediction of Artemisinin as an Anti-diabetic Candidate. *Reverse Docking*,

- Molecular Docking, Absorption, Distribution, and Toxicity Prediction of Artemisinin as an Anti-Diabetic Candidate*, 15(2), 88–96.
- Ruswanto. (2014). *Desain Dan Studi Interaksi Senyawa N'-(3,5-Dinitrobenzoyl)-Isonicotinohidrazide Pada Mycobacterium Tuberculosis Enoyl-Acyl Carrier Protein Reductase (Inha)*. 12(1), 1–10.
- Ruswanto, R., Mardianingrum, R., & Yanuar, A. (2022). Computational Studies of Thiourea Derivatives as Anticancer Candidates through Inhibition of Sirtuin-1 (SIRT1). *Jurnal Kimia Sains Dan Aplikasi*, 25(3), 87–96. <https://doi.org/10.14710/jksa.25.3.87-96>
- Ruswanto, R., Miftah, A. M., Tjahjono, D. H., & Siswandono. (2021). In silico study of 1-benzoyl-3-methylthiourea derivatives activity as epidermal growth factor receptor (EGFR) tyrosine kinase inhibitor candidates. *Chemical Data Collections*, 34(36), 100741. <https://doi.org/10.1016/j.cdc.2021.100741>
- Ruswanto, R., Nofianti, T., Mardianingrum, R., & Lestari, T. (2018). Desain dan Studi In Silico Senyawa Turunan Kuwanon-H sebagai Kandidat Obat Anti-HIV. *Jurnal Kimia VALENSI*, 4(1), 57–66. <https://doi.org/10.15408/jkv.v4i1.6867>
- Ruswanto, Setiawan, F., Rahayuningsih, N., Mardianingrum, R., Hidayati, N. L. D., & Eryanti, E. (2020). Synthesis, Characterization and In Silico Study of Fe(III) Complex with N'-(4-Chlorobenzoyl)-Isonicotino-Hydrazide as Anti Tuberculosis Candidate. *Jurnal Kimia Valensi*, 6(1), 69–80. <https://doi.org/10.15408/jkv.v6i1.11788>
- Sari, I. W., Junaidin, J., & Pratiwi, D. (2020). STUDI MOLECULAR DOCKING SENYAWA FLAVONOID HERBA KUMIS KUCING (Orthosiphon stamineus B.) Pada Reseptor A-Glukosidase Sebagai Antidiabetes Tipe 2. *Jurnal Farmagazine*, 7(2), 54. <https://doi.org/10.47653/farm.v7i2.194>
- Sawal, H. A., Nighat, S., Safdar, T., & Anees, L. (2023). Comparative In Silico Analysis and Functional Characterization of TANK-Binding Kinase 1–Binding Protein 1. *Bioinformatics and Biology Insights*, 17, 1–5. <https://doi.org/10.1177/11779322231164828>
- Scott A. Hollingsworth and Ron O. Dror. (2018). Molecular Dynamics simulation for all. *Neuron*, 176(3), 1–29. <https://doi.org/10.1016/j.neuron.2018.08.011>.Molecular
- Sung, H., Ferlay, J., Siegel, R. L., Laversanne, M., Soerjomataram, I., Jemal, A., & Bray, F. (2021). Global Cancer Statistics 2020: GLOBOCAN Estimates of Incidence and Mortality Worldwide for 36 Cancers in 185 Countries. *CA: A Cancer Journal for Clinicians*, 71(3), 209–249. <https://doi.org/10.3322/caac.21660>
- Yadav, N., Ganie, S. A., Singh, B., Chhillar, A. K., & Yadav, S. S. (2019). Phytochemical constituents and ethnopharmacological properties of *Ageratum conyzoides* L. *Phytotherapy Research*, 33(9), 2163–2178. <https://doi.org/10.1002/ptr.6405>