

DAFTAR PUSTAKA

- Abdullahi, M., & Adeniji, S. E. (2020). In-silico Molecular Docking and ADME/Pharmacokinetic Prediction Studies of Some Novel Carboxamide Derivatives as Anti-tubercular Agents. *Chemistry Africa*, 3(4), 989–1000. <https://doi.org/10.1007/s42250-020-00162-3>
- Ahmad, S., Khan, J. A., Kausar, T. N., Mahnashi, M. H., Alasiri, A., Alqahtani, A. A., Alqahtani, T. S., Walbi, I. A., Alshehri, O. M., & Elnoubi, O. A. (2023). Preparation, characterization and evaluation of flavonolignan silymarin effervescent floating matrix tablets for enhanced oral bioavailability. *Molecules*, 28(6), 2606. <https://doi.org/10.3390/molecules28062606>
- Aier, I., Varadwaj, P. K., & Raj, U. (2016). Structural insights into conformational stability of both wild-type and mutant EZH2 receptor. *Scientific Reports*, 6(1), 34984. <https://doi.org/10.1038/srep34984>
- Akbor, S., Bappi, M. H., Prottay, A. A. S., Haque, F., Mia, N., Islam, T., Almarhoon, Z. M., Güre, E. S., Setzer, W. N., Sharifi-Rad, J., Al Hasan, S., & Torequl Islam, M. (2025). Thymol as a Potential Natural Antiemetic: Insights From In Vivo and In Silico Studies. *Food Science & Nutrition*, 13(9), e70832. <https://doi.org/10.1002/fsn3.70832>
- Alghamdi, A., Abouzied, A. S., Alamri, A., Anwar, S., Ansari, M., Khadra, I., Zaki, Y. H., & Gomha, S. M. (2023). Synthesis, molecular docking, and dynamic simulation targeting main protease (Mpro) of new, thiazole clubbed pyridine scaffolds as potential COVID-19 inhibitors. *Current Issues in Molecular Biology*, 45(2), 1422–1442. <https://doi.org/10.3390/cimb45020093>
- Arnittali, M., Rissanou, A. N., & Harmandaris, V. (2019). Structure of biomolecules through molecular dynamics simulations. *Procedia Computer Science*, 156, 69–78. <https://doi.org/10.1016/j.procs.2019.08.181>
- Ayodele, P. F., Bamigbade, A., Bamigbade, O. O., Adeniyi, I. A., Tachin, E. S., Seweje, A. J., & Farohunbi, S. T. (2023). Illustrated procedure to perform molecular docking using PyRx and Biovia discovery studio visualizer: A case study of 10kt with atropine. *Progress in Drug Discovery & Biomedical Science*, 6(1). <https://hh-publisher.com/ojs321/index.php/pddb/article/view/877>
- Benet, L. Z., Hosey, C. M., Ursu, O., & Oprea, T. I. (2016). BDDCS, the Rule of 5 and drugability. *Advanced Drug Delivery Reviews*, 101, 89–98. <https://doi.org/10.1016/j.addr.2016.05.007>
- Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. N., & Bourne, P. E. (2021). The Protein Data Bank. *Nucleic Acids Research*, 28(1), 235–242. <https://doi.org/10.1093/nar/28.1.235>

- Cahyaningtias, R., Mirza, D. M., & Tilaqza, A. (2025). Simulasi molecular docking aktivitas antiinflamasi ekstrak metanol kulit buah matoa (*pometia pinnata*) sebagai inhibitor fosfolipase A2 dan prostaglandin D2. *Jurnal Bio Komplementer Medicine*, 12(1). <https://jim.unisma.ac.id/index.php/jbm/article/view/28464>
- Daina, A., & Zoete, V. (2016). A BOILED-Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. *ChemMedChem*, 11(11), 1117–1121. <https://doi.org/10.1002/cmdc.201600182>
- Ediz, E. F., & Kars, M. D. (n.d.). Molecular Docking Analysis of Thymoquinone and Thymol on Histamine Receptors. *Necmettin Erbakan Üniversitesi Fen ve Mühendislik Bilimleri Dergisi*, 7(1), 1–11. <https://doi.org/10.47112/neufmbd.2025.70>
- Engevik, A. C., Kaji, I., & Goldenring, J. R. (2020). The Physiology of the Gastric Parietal Cell. *Physiological Reviews*, 100(2), 573–602. <https://doi.org/10.1152/physrev.00016.2019>
- Fatriansyah, J. F., Rizqillah, R. K., Yandi, M. Y., & Sahlan, M. (2022). Molecular docking and dynamics studies on propolis sulabiroin-A as a potential inhibitor of SARS-CoV-2. *Journal of King Saud University-Science*, 34(1), 101707. <https://doi.org/10.1016/j.jksus.2021.101707>
- Fauziah, A., Fatharani, A., Nurawaliah, C. M., Rivianto, F. A., Sakina, I. V., Rahmawati, M., & Nurfadhila, L. (2023). Molecular docking senyawa yang berpotensi sebagai antikanker payudara: Literature review. *Journal of Pharmaceutical and Sciences*, 416–427. <https://doi.org/10.36490/journal-jps.com.v6i2.34>
- Forli, S., Huey, R., Pique, M. E., Sanner, M. F., Goodsell, D. S., & Olson, A. J. (2016). Computational protein-ligand docking and virtual drug screening with the AutoDock suite. *Nature Protocols*, 11(5), 905–919. <https://doi.org/10.1038/nprot.2016.051>
- Haider, Z., Subhani, M. M., Farooq, M. A., Ishaq, M., Khalid, M., Khan, R. S. A., & Niazi, A. K. (2020). In Silico discovery of novel inhibitors against main protease (Mpro) of SARS-CoV-2 using pharmacophore and molecular docking based virtual screening from ZINC database. *Preprint*, 10. <https://www.academia.edu/download/91826447/download.pdf>
- Hannan, M. A., Rahman, M. A., Sohag, A. A. M., Uddin, M. J., Dash, R., Sikder, M. H., Rahman, M. S., Timalisina, B., Munni, Y. A., Sarker, P. P., Alam, M., Mohibbullah, M., Haque, M. N., Jahan, I., Hossain, M. T., Afrin, T., Rahman, M. M., Tahjib-Ul-Arif, M., Mitra, S., ... Kim, B. (2021). Black Cumin (*Nigella sativa* L.): A Comprehensive Review on Phytochemistry, Health Benefits, Molecular Pharmacology, and Safety. *Nutrients*, 13(6), 1784. <https://doi.org/10.3390/nu13061784>

- Herman, R. (2019). Studi in Silico Lima Senyawa Aktif Sebagai Penghambat Protein Virus Dengue. *Jurnal Kefarmasian Indonesia*, 40–47. <https://doi.org/10.22435/jki.v9i1.1157>
- Hollingsworth, S. A., & Dror, R. O. (2018). Molecular dynamics simulation for all. *Neuron*, 99(6), 1129–1143. <https://doi.org/10.1016/j.neuron.2018.08.011>
- Ischak, N. I., Hasan, H., La Kilo, A., & Asnawi, A. (2023). In silico screening of *Andrographis paniculata* secondary metabolites as anti-diabetes mellitus through PDE9 inhibition. *Research in Pharmaceutical Sciences*, 18(1), 100–111. <https://doi.org/10.4103/1735-5362.363616>
- Jaghoori, M. M., Bleijlevens, B., & Olabarriaga, S. D. (2016). 1001 Ways to run AutoDock Vina for virtual screening. *Journal of Computer-Aided Molecular Design*, 30(3), 237–249. <https://doi.org/10.1007/s10822-016-9900-9>
- Kemenkes, R. I. (2019). *Sebelas Ramuan Jamu Saintifik Pemanfaatan Mandiri Oleh Masyarakat. Balai Besar Penelitian Dan Pengembangan Tanaman Obat Dan Obat Tradisional.*
- Khanal, P., Mandar, B. K., Patil, B. M., & Hullatti, K. K. (2019). In silico antidiabetic screening of borapetoside C, cordifolioside A and magnoflorine. *Indian J Pharm Sci*, 81(3), 550–555. [10.36468/pharmaceutical-sciences.543](https://doi.org/10.36468/pharmaceutical-sciences.543)
- Kržan, M., Keuschler, J., Mavri, J., & Vianello, R. (2020). Relevance of Hydrogen Bonds for the Histamine H2 Receptor-Ligand Interactions: A Lesson from Deuteration. *Biomolecules*, 10(2), 196. <https://doi.org/10.3390/biom10020196>
- Kumar, S., Plotnikov, N. V., Rouse, J. C., & Singh, S. K. (2018). Biopharmaceutical Informatics: Supporting biologic drug development via molecular modelling and informatics. *The Journal of Pharmacy and Pharmacology*, 70(5), 595–608. <https://doi.org/10.1111/jphp.12700>
- Magdy, M.-A., Hanan, E.-A., & Nabila, E.-M. (2012). Thymoquinone: Novel gastroprotective mechanisms. *European Journal of Pharmacology*, 697(1–3), 126–131. <https://doi.org/10.1016/j.ejphar.2012.09.042>
- Medić, B., Babić, Ž., Banić, M., & Ljubičić, L. (2021). MODERN APPROACH TO DYSPEPSIA. *Acta Clinica Croatica*, 60(4), 731–738. <https://doi.org/10.20471/acc.2021.60.04.21>
- Naufa, F., Mutiah, R., Yen, Y., & Indrawijaya, A. (2022). Studi in silico potensi senyawa katekin teh hijau (*Camellia sinensis*) sebagai antivirus SARS CoV-2 terhadap spike glycoprotein (6LZG) dan main protease (5R7Y). *J. Food Pharm. Sci*, 10(1), 584–596. www.journal.ugm.ac.id/v3/JFPA

- Niveshika, Verma, E., Maurya, S. K., Mishra, R., & Mishra, A. K. (2017). The combined use of in silico, in vitro, and in vivo analyses to assess anti-cancerous potential of a bioactive compound from Cyanobacterium Nostoc sp. MGL001. *Frontiers in Pharmacology*, 8, 873. <https://doi.org/10.3389/fphar.2017.00873>
- Nugraha, G., & Istyastono, E. P. (2021). Virtual target construction for structure-based screening in the discovery of histamine H2 receptor ligands. *International Journal of Applied Pharmaceutics*, 13(3). <https://pdfs.semanticscholar.org/9dd5/0decc5159674194b2c4a2214fb8d5f68090a.pdf>
- Nurlailiyah, F. A., Dwijayanti, D. R., Hermanto, F. E., Masruri, M., & Widodo, N. (2025). Cytotoxicity of Blumea balsamifera on A549 Lung Cancer Cells: Integrating in Vitro Analysis with Computational Study of AKT-1 Inhibition. *Tropical Journal of Natural Product Research*, 9(2). <https://doi.org/10.26538/tjnpr/v9i2.12>
- Oktaviana, L., Moulana, M. Z., Rusdin, A., Lestari, M. A., Fathin, N. M., & Novitasari, D. (2024). Senyawa bioaktif dari daun miana sebagai kandidat penghambat beta-laktamase: Studi Komputasi. *Jurnal Insan Farmasi Indonesia*, 7(3), 291–302. <https://doi.org/10.36387/392s0e44>
- Pantsar, T., & Poso, A. (2018). Binding affinity via docking: Fact and fiction. *Molecules*, 23(8), 1899. <https://doi.org/10.3390/molecules23081899>
- Rastini, M. B. O., Giantari, N. K. M., Adnyani, K. D., & Laksmiani, N. P. L. (2019). Molecular docking aktivitas antikanker dari kuersetin terhadap kanker payudara secara in silico. *Jurnal Kimia*, 180. <https://doi.org/10.24843/JCHEM.2019.v13.i02.p09>
- Ribeiro, A. R. S., Diniz, P. B. F., Pinheiro, M. S., Albuquerque-Júnior, R. L. C., & Thomazzi, S. M. (2016). Gastroprotective effects of thymol on acute and chronic ulcers in rats: The role of prostaglandins, ATP-sensitive K(+) channels, and gastric mucus secretion. *Chemico-Biological Interactions*, 244, 121–128. <https://doi.org/10.1016/j.cbi.2015.12.004>
- Rijal, S., Miskad, U. A., Achmad, D., Masadah, R., Daud, D., Kaelan, C., Rahawarin, H., Paramita, S., & Yasir, Y. (2016). Evaluation of Anti-ulcerogenic Activity in Oil Extract of Jintan Hitam (Nigella sativa) Against Ethanol Induced Gastric Ulcer in Mice (Mus musculus). *American Journal of Clinical and Experimental Medicine*, 4(6), 179–184. <https://doi.org/10.11648/j.ajcem.20160406.14>
- Rosa, F. L. (2023). Studi pendekatan molekuler modeling senyawa golongan flavonoid sebagai antiulcer pada tukak lambung. *Lambung Mangkurat Medical Seminar*, 4(1), 605–622. <https://fk.ulm.ac.id/ojs/index.php/lummens/article/download/243/219>

- 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), 54–60. <https://doi.org/10.47653/farm.v7i2.194>
- Semaoui, M., Mesli, F., Dib, M. E. A., Tabti, B., Achiri, R., Costa, J., & Muselli, A. (2022). Statistical analysis/theoretical investigations of novel vascular endothelial growth factor of Davanoide from *Scolymus grandifloras* Desf as potent anti-angiogenic drug properties. *Journal of Biomolecular Structure & Dynamics*, 40(9), 3850–3870. <https://doi.org/10.1080/07391102.2020.1851301>
- Siregar, G. P., Parwati, I., Tjahjodjati, T., Safriadi, F., Situmorang, G. R., Yohana, R., & Khairani, A. F. (2025). Molecular Dynamic Stability Study of VEGF Inhibitor in Patients with Bladder Cancer. *Acta Informatica Medica: AIM: Journal of the Society for Medical Informatics of Bosnia & Herzegovina: Casopis Drustva Za Medicinsku Informatiku BiH*, 33(1), 50–53. <https://doi.org/10.5455/aim.2024.33.50-53>
- Suleyman, H., Albayrak, A., Bilici, M., Cadirci, E., & Halici, Z. (2010). Different Mechanisms in Formation and Prevention of Indomethacin-induced Gastric Ulcers. *Inflammation*, 33(4), 224–234. <https://doi.org/10.1007/s10753-009-9176-5>
- Tabassum, H., & Ahmad, I. Z. (2021). Molecular Docking and Dynamics Simulation Analysis of Thymoquinone and Thymol Compounds from *Nigella sativa* L. that Inhibit Cag A and Vac A Oncoprotein of *Helicobacter pylori*: Probable Treatment of *H. pylori* Infections. *Medicinal Chemistry (Sharīqah (United Arab Emirates))*, 17(2), 146–157. <https://doi.org/10.2174/1573406416666200302113729>
- Ummah, K., Mahardika, R. G., & Mardiyah, A. (2020). Sintesis Senyawa Vanilil Metil Keton dan Uji Aktivitas Antiinflamasi terhadap Enzim COX-1 dan COX-2 melalui Analisis In Silico. *ALCHEMY: Journal of Chemistry*, 8(2), 1–11. <https://doi.org/10.18860/al.v8i2.10863>
- Wijarnpreecha, K., Panjawatnan, P., Leelasinjaroen, P., & Ungprasert, P. (2020). Statins and risk of peptic ulcer disease: A systematic review and meta-analysis. *Arab Journal of Gastroenterology: The Official Publication of the Pan-Arab Association of Gastroenterology*, 21(3), 135–138. <https://doi.org/10.1016/j.ajg.2020.07.007>
- Windari, T. (2017). Peranan ekstrak bawang dayak (*Eleutherine palmifolia*) sebagai agen anti tukak lambung (peptic ulcer) pada Tikus Wistar (*Rattus norvegicus*) jantan yang diinduksi etanol. *Jurnal Pangan Dan Agroindustri*, 5(1). <https://jpa.ub.ac.id/index.php/jpa/article/view/498>
- Xiong, G., Wu, Z., Yi, J., Fu, L., Yang, Z., Hsieh, C., Yin, M., Zeng, X., Wu, C., Lu, A., Chen, X., Hou, T., & Cao, D. (2021). ADMETlab 2.0: An integrated

- online platform for accurate and comprehensive predictions of ADMET properties. *Nucleic Acids Research*, 49(W1), W5–W14. <https://doi.org/10.1093/nar/gkab255>
- Yadav, S., & Chandra, A. (2020). Solvation Shell of the Nitrite Ion in Water: An Ab Initio Molecular Dynamics Study. *The Journal of Physical Chemistry B*, 124(33), 7194–7204. <https://doi.org/10.1021/acs.jpcb.0c02221>
- Zainuri, W., Azzahra, M. F., & Sukiman, A. (2024). Analisis Senyawa Kurkumin Pada Tanaman Kunyit (*Curcuma Longa*) Sebagai Obat Herbal Gastritis Menggunakan Analisis Pass, Swiss Adme Dan Docking. *Jurnal Biologi Dan Pembelajarannya (JB&P)*, 11(2), 161–172. <https://doi.org/10.29407/jbp.v11i2.22527>
- Zhang, J., Qi, T., & Wei, J. (2012). Homology modeling and antagonist binding site study of the human histamine H2 receptor. *Medicinal Chemistry (Shariqah (United Arab Emirates))*, 8(6), 1084–1092. <https://doi.org/10.2174/1573406411208061084>
- Zikri, A. T., Pranowo, H. D., & Haryadi, W. (2020). Stability, hydrogen bond occupancy analysis and binding free energy calculation from flavonol docked in DAPK1 active site using molecular dynamic simulation approaches. *Indonesian Journal of Chemistry*, 21(2), 383–390. <https://doi.org/10.22146/ijc.56087>
- Zubair, M. S., Maulana, S., & Mukaddas, A. (2020). Penambatan molekuler dan simulasi dinamika molekuler senyawa dari genus *nigella* terhadap penghambatan aktivitas enzim protease HIV-1. *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy)(e-Journal)*, 6(1), 132–140. <https://doi.org/10.22487/j24428744.2020.v6.i1.14982>
- Zuhroh, N., Rasmiyana, R., & Rachmawati, Y. (2025). Potensi Senyawa Timokuinon, Timol, dan Karvakrol dari Jintan Hitam (*Nigella sativa*) sebagai Agen Antibakteri Alami dalam Keamanan Pangan: Analisis In Silico terhadap *Escherichia coli* dan *Salmonella*. *Jurnal Teknologi Pangan Dan Industri Perkebunan (LIPIDA)*, 5(1), 26–33. <http://jurnal.politap.ac.id/index.php/lipida>