

DAFTAR PUSTAKA

- Adcock, S. A., & McCammon, J. A. (2006). Molecular dynamics: Survey of methods for simulating the activity of proteins. *Chemical Reviews*, 106(5), 1589–1615. <https://doi.org/10.1021/cr040426m>
- Ahmad, F., Cherukuri, M. K., & Choyke, P. L. (2021). Metabolic reprogramming in prostate cancer. *British Journal of Cancer*, 125(9), 1185–1196. <https://doi.org/10.1038/s41416-021-01435-5>
- Al-Fayez, S., & El-Metwally, A. (2023). Cigarette smoking and prostate cancer: A systematic review and meta-analysis of prospective cohort studies. *Tobacco Induced Diseases*, 21, 1–12. <https://doi.org/10.18332/tid/157231>
- Al-Ghazawi, M., Salameh, H., Amo-Afful, S., Khasawneh, S., & Ghanem, R. (2023). An In-Depth Look Into the Epidemiological and Etiological Aspects of Prostate Cancer: A Literature Review. *Cureus*, 15(11). <https://doi.org/10.7759/cureus.48252>
- American Cancer Society. (2016). Prostate Cancer What is prostate cancer ? *American Cancer Society*, 88.
- Astalakshmi, D. ., T, G., K B, G. S., M, N., M R, H. H. S., S, G., Latha, D. S. ., & Kumar, D. M. S. (2022). Over View on Molecular Docking: A Powerful Approach for Structure Based Drug Discovery. *International Journal of Pharmaceutical Sciences Review and Research*, 77(2), 146–157. <https://doi.org/10.47583/ijpsrr.2022.v77i02.029>
- Bagrodia, A., DiBlasio, C., Wake, R., & Derweesh, I. (2009). Adverse effects of androgen deprivation therapy in prostate cancer: Current management issues. *Indian Journal of Urology*, 25(2), 169–176. <https://doi.org/10.4103/0970-1591.52907>
- Bizuayehu, H. M., Ahmed, K. Y., Kibret, G. D., Dadi, A. F., Belachew, S. A., Bagade, T., Tegegne, T. K., Venchiarutti, R. L., Kibret, K. T., Hailegebireal, A. H., Assefa, Y., Khan, M. N., Abajobir, A., Alene, K. A., Mengesha, Z., Erku, D., Enquobahrie, D. A., Minas, T. Z., Misgan, E., & Ross, A. G. (2024). Global Disparities of Cancer and Its Projected Burden in 2050. *JAMA Network Open*, 7(11), e2443198. <https://doi.org/10.1001/jamanetworkopen.2024.43198>
- Bizuayehu, H. M., Dadi, A. F., Ahmed, K. Y., Tegegne, T. K., Hassen, T. A., Kibret, G. D., Ketema, D. B., Bore, M. G., Thapa, S., Odo, D. B., Kassa, Z. Y., Shifti, D. M., Amsalu, E., Sarich, P., Venchiarutti, R. L., Melaku, Y. A., Kibret, K. T., Habte, A., Mefsin, Y. M., ... Belachew, S. A. (2024). Burden of 30 cancers among men: Global statistics in 2022 and projections for 2050 using population-based estimates. *Cancer*, December 2023, 3708–3723.

<https://doi.org/10.1002/cncr.35458>

- Braun, E., Gilmer, J., Mayes, H. B., Mobley, D. L., Monroe, J. I., Prasad, S., & Zuckerman, D. M. (2019). Best Practices for Foundations in Molecular Simulations [Article v1.0]. *Living Journal of Computational Molecular Science*, 1(1). <https://doi.org/10.33011/livecoms.1.1.5957>
- Contreras-García, I. J., Cárdenas-Rodríguez, N., Romo-Mancillas, A., Bandala, C., Zamudio, S. R., Gómez-Manzo, S., Hernández-Ochoa, B., Mendoza-Torreblanca, J. G., & Pichardo-Macías, L. A. (2022). Levetiracetam Mechanisms of Action: From Molecules to Systems. *Pharmaceuticals*, 15(4). <https://doi.org/10.3390/ph15040475>
- Cosconati, S., Forli, S., Perryman, A. L., Harris, R., Goodsell, D. S., & Olson, A. J. (2010). Virtual screening with AutoDock: Theory and practice. *Expert Opinion on Drug Discovery*, 5(6), 597–607. <https://doi.org/10.1517/17460441.2010.484460>
- Culig, Z., & Santer, F. R. (2014). Androgen receptor signaling in prostate cancer. *Cancer and Metastasis Reviews*, 33(2–3), 413–427. <https://doi.org/10.1007/s10555-013-9474-0>
- Dictyotaceae, D. (2006). *Natural Product Communications Diterpenoid Constituents from the Brown Alga*.
- Dunn, M. W., & Kazer, M. W. (2011). Prostate cancer overview. *Seminars in Oncology Nursing*, 27(4), 241–250. <https://doi.org/10.1016/j.soncn.2011.07.002>
- El-Shaibany, A., Al-Habori, M., Al-Maqtari, T., & Al-Mahbashi, H. (2020). The Yemeni Brown Algae *Dictyota dichotoma* Exhibit High in Vitro Anticancer Activity Independent of Its Antioxidant Capability. *BioMed Research International*, 2020. <https://doi.org/10.1155/2020/2425693>
- Friedman, R., Nachliel, E., & Gutman, M. (2005). Molecular dynamics of a protein surface: Ion-residues interactions. *Biophysical Journal*, 89(2), 768–781. <https://doi.org/10.1529/biophysj.105.058917>
- Fujita, K., & Nonomura, N. (2019). Role of androgen receptor in prostate cancer: A review. *World Journal of Men's Health*, 37(3), 288–295. <https://doi.org/10.5534/wjmh.180040>
- Gallo, M. T., Grant, B. J., Teodoro, M. L., Melton, J., Cieplak, P., Phillips, G. N., & Stec, B. (2009). Novel procedure for thermal equilibration in molecular dynamics simulation. *Molecular Simulation*, 35(5), 349–357. <https://doi.org/10.1080/08927020802647272>
- Gao, L., Zhao, R., Liu, J., Zhang, W., Sun, F., Yin, Q., Wang, X., Wang, M., Feng,

- T., Qin, Y., Cai, W., Li, Q., Dong, H., Chen, X., Xiong, X., Liu, H., Hu, J., Chen, W., & Han, B. (2021). KIF15 Promotes Progression of Castration Resistant Prostate Cancer by Activating EGFR Signaling Pathway. *Frontiers in Oncology*, 11(November), 1–13. <https://doi.org/10.3389/fonc.2021.679173>
- Gasmi, A., Roubaud, G., Dariane, C., Barret, E., Beauval, J. B., Brureau, L., Créhange, G., Fiard, G., Fromont, G., Gauthé, M., Ruffion, A., Renard-Penna, R., Sargos, P., Rouprêt, M., Ploussard, G., & Mathieu, R. (2022). Overview of the development and use of Akt inhibitors in prostate cancer. *Journal of Clinical Medicine*, 11(1), 1–10. <https://doi.org/10.3390/jcm11010160>
- Halder, S. K., Sultana, I., Shuvo, M. N., Shil, A., Himel, M. K., Hasan, M. A., & Shawan, M. M. A. K. (2023). In Silico Identification and Analysis of Potentially Bioactive Antiviral Phytochemicals against SARS-CoV-2: A Molecular Docking and Dynamics Simulation Approach. *BioMed Research International*, 2023(May). <https://doi.org/10.1155/2023/5469258>
- Handle, F., Pühr, M., Gruber, M., Andolfi, C., Schäfer, G., Klocker, H., Haybaeck, J., De Wulf, P., & Culig, Z. (2023). The Oncogenic Protein Kinase/ATPase RIOK1 Is Up-Regulated via the c-myc/E2F Transcription Factor Axis in Prostate Cancer. *American Journal of Pathology*, 193(9), 1284–1297. <https://doi.org/10.1016/j.ajpath.2023.05.013>
- 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>
- Hassan, A. M., Gattan, H. S., Faizo, A. A., Alruhaili, M. H., Alharbi, A. S., Bajrai, L. H., AL-Zahrani, I. A., Dwivedi, V. D., & Azhar, E. I. (2024). Evaluating the Binding Potential and Stability of Drug-like Compounds with the Monkeypox Virus VP39 Protein Using Molecular Dynamics Simulations and Free Energy Analysis. *Pharmaceuticals*, 17(12). <https://doi.org/10.3390/ph17121617>
- He, Y., Xu, W., Xiao, Y. T., Huang, H., Gu, D., & Ren, S. (2022). Targeting signaling pathways in prostate cancer: mechanisms and clinical trials. *Signal Transduction and Targeted Therapy*, 7(1). <https://doi.org/10.1038/s41392-022-01042-7>
- Herrera-Rodríguez, A. M., Miletić, V., Aponte-Santamaría, C., & Gräter, F. (2019). Molecular Dynamics Simulations of Molecules in Uniform Flow. *Biophysical Journal*, 116(9), 1579–1585. <https://doi.org/10.1016/j.bpj.2018.12.025>
- Huang, F. K., Han, S., Xing, B., Huang, J., Liu, B., Bordeleau, F., Reinhart-King, C. A., Zhang, J. J., & Huang, X. Y. (2015). Targeted inhibition of fascin function blocks tumour invasion and metastatic colonization. *Nature Communications*,

- 6(May). <https://doi.org/10.1038/ncomms8465>
- Huang, S. Y., Grinter, S. Z., & Zou, X. (2010). Scoring functions and their evaluation methods for protein-ligand docking: Recent advances and future directions. *Physical Chemistry Chemical Physics*, 12(40), 12899–12908. <https://doi.org/10.1039/c0cp00151a>
- Imran, M., Iqbal, A., Badshah, S. L., Sher, A. A., Ullah, H., Ayaz, M., Mosa, O. F., Mostafa, N. M., & Daglia, M. (2023). Chemical and Nutritional Profiling of the Seaweed *Dictyota dichotoma* and Evaluation of Its Antioxidant, Antimicrobial and Hypoglycemic Potentials. *Marine Drugs*, 21(5). <https://doi.org/10.3390/md21050273>
- Kim, S., Thiessen, P. A., Bolton, E. E., Chen, J., Fu, G., Gindulyte, A., Han, L., He, J., He, S., Shoemaker, B. A., Wang, J., Yu, B., Zhang, J., & Bryant, S. H. (2016). PubChem substance and compound databases. *Nucleic Acids Research*, 44(D1), D1202–D1213. <https://doi.org/10.1093/nar/gkv951>
- Kolina, J., Sumiwi, S. A., & Levita, J. (2019). MODE IKATAN METABOLIT SEKUNDER DI TANAMAN AKAR KUNING (*Arcangelisia flava* L.) DENGAN NITRAT OKSIDA SINTASE. *FITOFARMAKA: Jurnal Ilmiah Farmasi*, 8(1), 45–52. <https://doi.org/10.33751/jf.v8i1.1171>
- Li, C., Cheng, D., & Li, P. (2025). Androgen receptor dynamics in prostate cancer: from disease progression to treatment resistance. *Frontiers in Oncology*, 15(February), 1–12. <https://doi.org/10.3389/fonc.2025.1542811>
- Lin, H. K., Wang, L., Hu, Y. C., Altuwaijri, S., & Chang, C. (2002). Phosphorylation-dependent ubiquitylation and degradation of androgen receptor by Akt require Mdm2 E3 ligase. *EMBO Journal*, 21(15), 4037–4048. <https://doi.org/10.1093/emboj/cdf406>
- Maftucha, N., Manalu, R., Amelia, R., Cordia, P., & Bupu, R. (2022). Potensi Senyawa Turunan Xanton dari Kulit Buah Manggis (*Garcinia mangostana* L.) Sebagai Inhibitor Protein Mycobacterium tuberculosis: Studi In Silico. *Pharmaceutical Journal of Indonesia*, 7, 123–128. <https://doi.org/10.21776/ub.pji.2022.007.02.7>
- Mehralivand, S., Thomas, C., Pühr, M., Claessens, F., van de Merbel, A. F., Dubrovskaya, A., Jenster, G., Bernemann, C., Sommer, U., & Erb, H. H. H. (2024). New advances of the androgen receptor in prostate cancer: report from the 1st International Androgen Receptor Symposium. *Journal of Translational Medicine*, 22(1), 1–8. <https://doi.org/10.1186/s12967-024-04878-5>
- Miceli, L. A., Teixeira, V. L., Castro, H. C., Rodrigues, C. R., Mello, J. F. R., Albuquerque, M. G., Cabral, L. M., De Brito, M. A., & De Souza, A. M. T.

- (2013). Molecular docking studies of marine diterpenes as inhibitors of wild-type and mutants HIV-1 reverse transcriptase. *Marine Drugs*, 11(11), 4127–4143. <https://doi.org/10.3390/md11114127>
- Mohanty, M., & Mohanty, P. S. (2023). Molecular docking in organic, inorganic, and hybrid systems: a tutorial review. *Monatshefte Fur Chemie*, 154(7), 683–707. <https://doi.org/10.1007/s00706-023-03076-1>
- Mohimani, H., Gurevich, A., Mikheenko, A., Garg, N., Nothias, L.-F., Ninomiya, A., Kentaro Takada, P. C. D., & Pevzner, P. A. (2017). Molecular Dynamics for all. *Physiology & Behavior*, 176(3), 139–148. <https://doi.org/10.1016/j.neuron.2018.08.011>.Molecular
- Morris, G. M., & Lim-Wilby, M. (2008). Molecular docking. *Methods in Molecular Biology*, 443, 365–382. https://doi.org/10.1007/978-1-59745-177-2_19
- Mullard, A. (2018). Re-assessing the rule of 5, two decades on. *Nature Reviews Drug Discovery*, 17(11), 777. <https://doi.org/10.1038/nrd.2018.197>
- Nada, H., Elkamhawy, A., & Lee, K. (2022). Identification of 1H-purine-2, 6-dione derivative as a potential SARS-CoV-2 main protease inhibitor: molecular docking, dynamic simulations, and energy calculations. *PeerJ*, 10, 1–30. <https://doi.org/10.7717/peerj.14120>
- Narayan, V., Ross, A. E., Parikh, R. B., Nohria, A., & Morgans, A. K. (2021). How to Treat Prostate Cancer With Androgen Deprivation and Minimize Cardiovascular Risk: A Therapeutic Tightrope. *JACC: CardioOncology*, 3(5), 737–741. <https://doi.org/10.1016/j.jacc.2021.09.014>
- Nittinger, E., Inhester, T., Bietz, S., Meyder, A., Schomburg, K. T., Lange, G., Klein, R., & Rarey, M. (2017). Large-Scale Analysis of Hydrogen Bond Interaction Patterns in Protein-Ligand Interfaces. *Journal of Medicinal Chemistry*, 60(10), 4245–4257. <https://doi.org/10.1021/acs.jmedchem.7b00101>
- Noor, F., Qamar, M. T. U., Ashfaq, U. A., Albutti, A., Alwashmi, A. S. S., & Aljasir, M. A. (2022). Network Pharmacology Approach for Medicinal Plants: Review and Assessment. *Pharmaceuticals*, 15(5), 1–33. <https://doi.org/10.3390/ph15050572>
- Oashi, T., Ringer, A. L., Raman, E. P., & MacKerell, A. D. (2011). Automated selection of compounds with physicochemical properties to maximize bioavailability and druglikeness. *Journal of Chemical Information and Modeling*, 51(1), 148–158. <https://doi.org/10.1021/ci100359a>
- Ofner, H., Kramer, G., Shariat, S. F., & Hassler, M. R. (2025). TP53 Deficiency in the Natural History of Prostate Cancer. *Cancers*, 17(4). <https://doi.org/10.3390/cancers17040645>

- Ormeño, F., & General, I. J. (2024). Convergence and equilibrium in molecular dynamics simulations. *Communications Chemistry*, 7(1), 1–11. <https://doi.org/10.1038/s42004-024-01114-5>
- Qian, H., Chen, B. B., Zhang, M., Zeng, S. J., Jia, Z. Z., Wang, S., Gao, S., Shi, A. H., & Xie, J. (2025). Network pharmacology and molecular docking approach to explore the potential mechanisms of Xuefu Zhuyu Capsule in coronary heart disease. *Medicine (United States)*, 104(1). <https://doi.org/10.1097/MD.00000000000041154>
- Rizvi, S. M., Shazi, S., & Mohd., H. (2013). A simple click by click protocol to perform docking : *EXCLI Journal*, 12, 831–857.
- Rushdi, M. I., Abdel-Rahman, I. A. M., Attia, E. Z., Saber, H., Saber, A. A., Bringmann, G., & Abdelmohsen, U. R. (2022). The Biodiversity of the Genus Dictyota: Phytochemical and Pharmacological Natural Products Prospectives. *Molecules*, 27(3), 1–30. <https://doi.org/10.3390/molecules27030672>
- Safi, R., Wardell, S. E., Watkinson, P., Qin, X., Lee, M., Park, S., Krebs, T., Dolan, E. L., Blattler, A., Tsuji, T., Nayak, S., Khater, M., Fontanillo, C., Newlin, M. A., Kirkland, M. L., Xie, Y., Long, H., Fink, E. C., Fanning, S. W., ... McDonnell, D. P. (2024). Androgen receptor monomers and dimers regulate opposing biological processes in prostate cancer cells. *Nature Communications*, 15(1), 1–19. <https://doi.org/10.1038/s41467-024-52032-y>
- Sahoo, R. N., Pattanaik, S., Pattnaik, G., Mallick, S., & Mohapatra, R. (2022). Review on the use of Molecular Docking as the First Line Tool in Drug Discovery and Development. *Indian Journal of Pharmaceutical Sciences*, 84(5), 1334–1337. <https://doi.org/10.36468/pharmaceutical-sciences.1031>
- Santamaria, R. (2023). Molecular dynamics. *Molecular Dynamics*, 1–385. <https://doi.org/10.1007/978-3-031-37042-7>
- Saurabh, S., Sivakumar, P. M., Perumal, V., Khosravi, A., Sugumaran, A., & Prabhawathi, V. (2020). Molecular Dynamics Simulations in Drug Discovery and Drug Delivery. *Engineering Materials*, 275–301. https://doi.org/10.1007/978-3-030-36260-7_10
- Scarpato, K. R., & Albertsen, P. C. (2016). Prostate-Specific Antigen Screening Guidelines. *Prostate Cancer: Science and Clinical Practice: Second Edition*, 9, 111–116. <https://doi.org/10.1016/B978-0-12-800077-9.00013-X>
- Sekhoacha, M., Riet, K., Motloun, P., Gumenku, L., Adegoke, A., & Mashele, S. (2022). Prostate Cancer Review: Genetics, Diagnosis, Treatment Options, and Alternative Approaches. *Molecules*, 27(17), 1–33. <https://doi.org/10.3390/molecules27175730>

- Siddiqui, Z. A., & Krauss, D. J. (2018). Adjuvant androgen deprivation therapy for prostate cancer treated with radiation therapy. *Translational Andrology and Urology*, 7(3), 378–389. <https://doi.org/10.21037/tau.2018.01.06>
- Singh, S., Bani Baker, Q., & Singh, D. B. (2021). Molecular docking and molecular dynamics simulation. *Bioinformatics: Methods and Applications*, 291–304. <https://doi.org/10.1016/B978-0-323-89775-4.00014-6>
- Siti, D., Hentu, R. M., Muchlisin, M. A., Jamil, A. S., Juni, E., & Rafikayanti, A. (2024). Potential Activity Of Secondary Metabolites Of Kawista (Limonia Acidissima) As Neurodegenerative Diseases : A Network Pharmacology Approaches. *Jurnal Eduhealth*, 15(02), 1246–1258. <https://doi.org/10.54209/eduhealth.v15i02>
- Song, X., Bao, L., Feng, C., Huang, Q., Zhang, F., Gao, X., & Han, R. (2024). Accurate Prediction of Protein Structural Flexibility by Deep Learning Integrating Intricate Atomic Structures and Cryo-EM Density Information. *Nature Communications*, 15(1), 1–14. <https://doi.org/10.1038/s41467-024-49858-x>
- Szklarczyk, D., Gable, A. L., Lyon, D., Junge, A., Wyder, S., Huerta-Cepas, J., Simonovic, M., Doncheva, N. T., Morris, J. H., Bork, P., Jensen, L. J., & Von Mering, C. (2019). STRING v11: Protein-protein association networks with increased coverage, supporting functional discovery in genome-wide experimental datasets. *Nucleic Acids Research*, 47(D1), D607–D613. <https://doi.org/10.1093/nar/gky1131>
- Tien, A. H., & Sadar, M. D. (2019). Keys to unlock androgen receptor translocation. *Journal of Biological Chemistry*, 294(22), 8711–8712. <https://doi.org/10.1074/jbc.H119.009180>
- Tzelepi, V. (2023). Prostate Cancer: Pathophysiology, Pathology and Therapy. *Cancers*, 15(1), 1–6. <https://doi.org/10.3390/cancers15010281>
- Vayalil, P. K. (2019). Mitochondrial oncobioenergetics of prostate tumorigenesis (Review). *Oncology Letters*, 18(5), 4367–4376. <https://doi.org/10.3892/ol.2019.10785>
- Wang, R., Qu, Z., Lv, Y., Yao, L., Qian, Y., Zhang, X., & Xiang, L. (2024). Important Roles of PI3K/AKT Signaling Pathway and Relevant Inhibitors in Prostate Cancer Progression. *Cancer Medicine*, 13(21), 1–11. <https://doi.org/10.1002/cam4.70354>
- Wang, Y., Xiao, J., Suzek, T. O., Zhang, J., Wang, J., & Bryant, S. H. (2009). PubChem: A public information system for analyzing bioactivities of small molecules. *Nucleic Acids Research*, 37(SUPPL. 2), 623–633.

<https://doi.org/10.1093/nar/gkp456>

- Wei, W., Cherukupalli, S., Jing, L., Liu, X., & Zhan, P. (2020). Fsp3: A new parameter for drug-likeness. *Drug Discovery Today*, 25(10), 1839–1845. <https://doi.org/10.1016/j.drudis.2020.07.017>
- Weni, M., Safithri, M., & Seno, D. S. H. (2020). Molecular Docking of Active Compounds Piper crocatum on The Alpha- Glucosidase Enzyme as Antidiabetic Penambatan Molekuler Senyawa Aktif Daun Sirih Merah (Piper Crocatum) terhadap Enzim Alfa-Glukosidase sebagai Antidiabetes. *Indonesian Journal of Pharmaceutical Science and Technology*, 7(2), 64–72.
- Widyasari, A. D., Nur Ramadhan, L. O. A., & Dewi, C. (2022). Pemodelan Farmakofor dan Skrining Virtual dari Database Senyawa Bahan Alam Sebagai Inhibitor Sars-CoV-2 RNA-dependent RNA Polimerase. *Jurnal Pharmacia Mandala Waluya*, 1(6), 247–257. <https://doi.org/10.54883/jpmw.v1i6.49>
- Yan, Z., Liu, R., Liu, B., Shao, Y., & Liu, M. (2023). Molecular Dynamics Simulation Studies of Properties, Preparation, and Performance of Silicon Carbide Materials: A Review. *Energies*, 16(3). <https://doi.org/10.3390/en16031176>
- Zhao, X., Xiu, J., Yang, H., Han, W., & Jin, Y. (2025). Network Pharmacology and Bioinformatics Study of Six Medicinal Food Homologous Plants Against Colorectal Cancer. *International Journal of Molecular Sciences*, 26(3), 1–18. <https://doi.org/10.3390/ijms26030930>