DAFTAR PUSTAKA

Abou Assi, R., Darwis, Y., Abdulbaqi, I. M., khan, A. A., Vuanghao, L., & Laghari, M. H. (2017). Morinda citrifolia (Noni): A comprehensive review on its industrial uses, pharmacological activities, and clinical trials. *Arabian Journal of Chemistry*, *10*(5), 691–707. https://doi.org/10.1016/j.arabjc.2015.06.018

Agrawal, N., Sharma, M., Singh, S., & Goyal, A. (2022). Recent Advances of α-Glucosidase Inhibitors: A Comprehensive Review. *Current Topics in Medicinal Chemistry*, *22*(25), 2069–2086. https://doi.org/10.2174/1568026622666220831092855

Agrawal, P., Singh, H., Srivastava, H. K., Singh, S., Kishore, G., & Raghava, G. P. S. (2019). Benchmarking of different molecular docking methods for protein-peptide docking. *BMC Bioinformatics*, *19*(Suppl 13). https://doi.org/10.1186/s12859-018-2449-y

Akbar, N.A., Amin, S.,& Wulandari, W. T. (2022). Studi In Silico Senyawa Yang Terkandung Dalam Tanaman Daun Sirih Merah (Piper Crocatum RUIZ & PAV) Sebagai Kandidat Anti SARS CoV-2. *Ejurnal Universitas Bth*, *2*, 378–391. https://repository.universitas-bth.ac.id/2246/%0Ahttps://repository.universitas-bth.ac.id/2246/3/DAFTAR PUSTAKA.pdf

Alam, Q. (2023). Molecular Docking Analysis Of AGTR1 Antagonists. *Bioinformation*, *19*(3), 284–289. https://doi.org/10.6026/97320630019284

Ali, F., Wali, H., Jan, S., Zia, A., Aslam, M., Ahmad, I., Afridi, S. G., Shams, S., & Khan, A. (2021). Analysing the essential proteins set of Plasmodium falciparum PF3D7 for novel drug targets identification against malaria. *Malaria Journal*, *20*(1), 1–11. https://doi.org/10.1186/s12936-021-03865-1

Almeida, É. S., de Oliveira, D., & Hotza, D. (2019). Properties and Applications of Morinda Citrifolia (Noni): A Review. *Comprehensive Reviews in Food Science and Food Safety*, *00*, 1–27. https://doi.org/10.1111/1541-4337.12456

B. Fernandes, T., C. F. Segretti, M., C. Polli, M., & Parise-Filho, R. (2016). Analysis of the Applicability and Use of Lipinski`s Rule for Central Nervous System Drugs. *Letters in Drug Design & Discovery*, *13*(10), 999–1006. https://doi.org/10.2174/1570180813666160622092839

Bié, J., Sepodes, B., Fernandes, P. C. B., & Ribeiro, M. H. L. (2023). Polyphenols in Health and Disease: Gut Microbiota, Bioaccessibility, and Bioavailability. *Compounds*, *3*(1), 40–72. https://doi.org/10.3390/compounds3010005

Burley, S. K., Berman, H. M., Bhikadiya, C., Bi, C., Chen, L., Di Costanzo, L., Christie, C., Duarte, J. M., Dutta, S., Feng, Z., Ghosh, S., Goodsell, D. S., Green, R. K., Guranovic, V., Guzenko, D., Hudson, B. P., Liang, Y., Lowe, R., Peisach, E., … Ioannidis, Y. E. (2019). Protein Data Bank: The single global archive for 3D macromolecular structure data. *Nucleic Acids Research*,

47(D1), D520–D528. https://doi.org/10.1093/nar/gky949

Carrillo-López, A., & Yahia, E. M. (2011). Noni (Morinda citrifolia L.). *Postharvest Biology and Technology of Tropical and Subtropical Fruits*, *4*(May). https://doi.org/10.1533/9780857092618.51

Case, D. A., Aktulga, H. M., Belfon, K., Cerutti, D. S., Cisneros, G. A., Cruzeiro, V. W. D., Forouzesh, N., Giese, T. J., Götz, A. W., Gohlke, H., Izadi, S., Kasavajhala, K., Kaymak, M. C., King, E., Kurtzman, T., Lee, T. S., Li, P., Liu, J., Luchko, T., … Merz, K. M. (2023). AmberTools. *Journal of Chemical Information and Modeling*. https://doi.org/10.1021/acs.jcim.3c01153

Chagas, C. M., Moss, S., & Alisaraie, L. (2018). Drug metabolites and their effects on the development of adverse reactions: Revisiting Lipinski's Rule of Five. *International Journal of Pharmaceutics*, *549*(1–2), 133–149. https://doi.org/10.1016/j.ijpharm.2018.07.046

Christian Baber, J., Thompson, D. C., Cross, J. B., & Humblet, C. (2009). GARD: A generally applicable replacement for RMSD. *Journal of Chemical Information and Modeling*, *49*(8), 1889–1900. https://doi.org/10.1021/ci9001074

Das, S., Sarmah, S., Lyndem, S., & Singha Roy, A. (2021). An Investigation Into The Identification of Potential Inhibitors of SARS-CoV-2 Main Protease Using Molecular Docking Study. *Journal of Biomolecular Structure and Dynamics*, *39*(9), 3347–3357. https://doi.org/10.1080/07391102.2020.1763201

Davis, A. M., Teague, S. J., & Kleywegt, G. J. (2003). Application and limitations of x-ray crystallographic data in structure-based ligand and drug design. *Angewandte Chemie - International Edition*, *42*(24), 2718–2736. https://doi.org/10.1002/anie.200200539

Dirir, A. M., Daou, M., Yousef, A. F., & Yousef, L. F. (2022). A Review Of Alpha-Glucosidase Inhibitors From Plants As Potential Candidates For The Treatment Of Type-2 Diabetes. In *Phytochemistry Reviews* (Vol. 21, Issue 4). Springer Netherlands. https://doi.org/10.1007/s11101-021-09773-1

Donati, L., Weber, M., & Fackeldey, K. (2023). *PLANTS+: Improving Ant Colony Algorithms for Drug Design*. 0–21. https://doi.org/10.21203/rs.3.rs-2747350/v1

Dulsat, J., López-Nieto, B., Estrada-Tejedor, R., & Borrell, J. I. (2023). Evaluation of Free Online ADMET Tools for Academic or Small Biotech Environments. *Molecules*, *28*(2). https://doi.org/10.3390/molecules28020776

Elahabaadi, E., Salarian, A. A., & Nassireslami, E. (2022). Design, Synthesis, and Molecular Docking of Novel Hybrids of Coumarin-Dithiocarbamate Alpha-Glucosidase Inhibitors Targeting Type 2 Diabetes Mellitus. *Polycyclic Aromatic Compounds*, *42*(7), 4317–4327. https://doi.org/10.1080/10406638.2021.1887295

Endriyatno, N. C., & Walid, M. (2022). Studi In Silico Kandungan Senyawa Daun

Srikaya (Annona squamosa L.)Terhadap Protein Dihydrofolate Reductase Pada Mycobacterium tuberculosis. *Pharmacon: Jurnal Farmasi Indonesia*, *19*(1), 87–98. https://doi.org/10.23917/pharmacon.v19i1.18044

Faridah, Esti Mumpuni, Y. I. Y. (2019). *Pandangan Analisis In-silico Senyawa Kimia dalam Teh Hijau Bekerja pada Aktivator PPAR-γ sebagai Antiobesitas.pdf*. JURNAL ILMU KEFARMASIAN INDONESIA.

Galicia-Garcia, U., Benito-Vicente, A., Jebari, S., Larrea-Sebal, A., Siddiqi, H., Uribe, K. B., Ostolaza, H., & Martín, C. (2020). Pathophysiology of Type 2 Diabetes Mellitus. *International Journal of Molecular Sciences*, *21*(17), 1–34. https://doi.org/10.3390/ijms21176275

Gendokesumo, M. E., Putra, G. S., Anwari, F., Widianat, W., & Elysia, M. (2022). Studi In-Silico Menghambat Enzim α-Glukosidase Pada Fitokimia Yang Terkandung Pada Momordica Charantia Linn. (Pare) Sebagai Terapi Diabetes. *Akta Kimia Indonesia*, *7*(1), 77. https://doi.org/10.12962/j25493736.v7i1.12588

Hardianto, D. (2021). Telaah Komprehensif Diabetes Melitus: Klasifikasi, Gejala, Diagnosis, Pencegahan, Dan Pengobatan. *Jurnal Bioteknologi & Biosains Indonesia (JBBI)*, *7*(2), 304–317. https://doi.org/10.29122/jbbi.v7i2.4209

Hayet, S., Sujan, K. M., Mustari, A., & Miah, M. A. (2021). Hemato-biochemical profile of turkey birds selected from Sherpur district of Bangladesh. *Int. J. Adv. Res. Biol. Sci*, *8*(6), 1–5. https://doi.org/10.22192/ijarbs

Hedrington, M. S., & Davis, S. N. (2019). Considerations When Using Alpha-Glucosidase Inhibitors In The Treatment of Type 2 Diabetes. *Expert Opinion on Pharmacotherapy*, *20*(18), 2229–2235. https://doi.org/10.1080/14656566.2019.1672660

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

International Diabetes Federation. (2021). IDF Diabetes Atlas 2021 _ IDF Diabetes Atlas. In *IDF official website*. https://diabetesatlas.org/atlas/tenth-edition/%0Ahttps://diabetesatlas.org/data/en/world/

Joshi, H., Li, C. Y., & Aksimentiev, A. (2023). All-Atom Molecular Dynamics Simulations of Membrane-Spanning DNA Origami Nanopores. *Methods in Molecular Biology*, *2639*, 113–128. https://doi.org/10.1007/978-1-0716-3028-0_7

Kelutur, F. J., Mustarichie, R., & Umar, A. K. (2020). Virtual Screening Kandungan Senyawa Kipas Laut (Gorgonia mariae) Sebagai Anti-Asma. *ALCHEMY Jurnal Penelitian Kimia*, *16*(2), 48. https://doi.org/10.20961/alchemy.16.2.39965.48-59

Keresztes, P., & Peacock-Johnson, A. (2019). CE: Type 2 Diabetes: A Pharmacologic Update. *American Journal of Nursing*, *119*(3), 32–40. https://doi.org/10.1097/01.NAJ.0000554008.77013.cf

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

Khasanah, N. U., Wardani, G. A., & Mardianingrum, R. (2023). *Jurnal Kimia Sains dan Aplikasi 3-Phenylthiourea) Cobalt (III) as Anticancer Candidate*. *26*(7), 238–248.

Kumar, S., Sharma, P. P., Shankar, U., Kumar, D., Joshi, S. K., Pena, L., Durvasula, R., Kumar, A., Kempaiah, P., Poonam, & Rathi, B. (2020). Discovery of New Hydroxyethylamine Analogs against 3CLproProtein Target of SARS-CoV-2: Molecular Docking, Molecular Dynamics Simulation, and Structure-Activity Relationship Studies. *Journal of Chemical Information and Modeling*, *60*(12), 5754–5770. https://doi.org/10.1021/acs.jcim.0c00326

Lin, Y. T., Lin, H. R., Yang, C. S., Liaw, C. C., Sung, P. J., Kuo, Y. H., Cheng, M. J., & Chen, J. J. (2022). Antioxidant and Anti-α-Glucosidase Activities of Various Solvent Extracts and Major Bioactive Components From the Fruits of Crataegus Pinnatifida. *Antioxidants*, *11*(2), 1–16. https://doi.org/10.3390/antiox11020320

Lohani, M., Majrashi, M., Govindarajulu, M., Patel, M., Ramesh, S., Bhattacharya, D., Joshi, S., Fadan, M., Nadar, R., Darien, B., Maurice, D. V., Kemppainen, B., & Dhanasekaran, M. (2019). Immunomodulatory Actions Of a Polynesian Herb Noni (Morinda citrifolia) and its Clinical Applications. *Complementary Therapies in Medicine*, *47*(September). https://doi.org/10.1016/j.ctim.2019.102206

Manalu, R. (2021). Docking Molekuler Senyawa Aktif Buah dan DaunJambu Biji (Psidium guajava L.) Terhadap Potein SARS-CoV-2. In *Forte Journal* (Vol. 1, Issue 2, pp. 77–84). https://doi.org/10.51771/fj.v1i2.89

Mardiana, M., & Ruswanto. (2019). Simulasi Dinamika Molekular Senyawa Pyridin Pada Protein 2XNB. *Research Gate*, *9*(5), 1–15.

Maria Angelina Genere Koban, Sri Rahayu Lestari, & Frida Kunti Setiowati. (2022). Analisis In Silico Naringenin dari Umbi Akar Batu (Gerrardanthus macrorhizus Harv.ex Benth. & Hook.f.) sebagai Antitusif terhadap Reseptor N-methyl-D-aspartate. *Biota : Jurnal Ilmiah Ilmu-Ilmu Hayati*, *7*(3), 172–182. https://doi.org/10.24002/biota.v7i3.5912

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

Morze, J., Wittenbecher, C., Schwingshackl, L., Danielewicz, A., Rynkiewicz, A., Hu, F. B., & Guasch-Ferre, M. (2022). Metabolomics and Type 2 Diabetes Risk: An Updated Systematic Review and Meta-analysis of Prospective Cohort Studies. *Diabetes Care*, *45*(4), 1013–1024.

https://doi.org/10.2337/dc21-1705

Mulatsari, E., Mumpuni, E., & Ramadhan, I. (2019). Skrining Virtual dan Elusidasi Moda Ikatan Senyawa dalam Bawang Putih (Allium Sativum L.) sebagai Penghambat Reseptor Advanced Glycation end Products. *Jurnal Ilmu Kefarmasian Indonesia*, *17*(2), 210. https://doi.org/10.35814/jifi.v17i2.749

Muttaqin, F. Z. (2019). Studi Molecular Docking, Molecular Dynamic, Dan Prediksi Toksisitas Senyawa Turunan Alkaloid Naftiridin Sebagai Inhibitor Protein Kasein Kinase 2-A Pada Kanker Leukemia. *Pharmacoscript*, *2*(1), 49–64. https://doi.org/10.36423/pharmacoscript.v2i1.241

Mvondo, J. G. M., Matondo, A., Mawete, D. T., Bambi, S.-M. N., Mbala, B. M., & Lohohola, P. O. (2021). In Silico ADME/T Properties of Quinine Derivatives Using SwissADME and pkCSM Webservers. *International Journal of TROPICAL DISEASE & Health*, *August*, 1–12. https://doi.org/10.9734/ijtdh/2021/v42i1130492

Nerurkar, P. V., Hwang, P. W., & Saksa, E. (2015). Anti-Diabetic Potential Of Noni: The Yin and The Yang. In *Molecules* (Vol. 20, Issue 10). https://doi.org/10.3390/molecules201017684

Ogle, G. D., James, S., Dabelea, D., Pihoker, C., Svennson, J., Maniam, J., Klatman, E. L., & Patterson, C. C. (2022). Global Estimates Of Incidence Of Type 1 Diabetes In Children And Adolescents: Results Trom The International Diabetes Federation Atlas, 10th edition. *Diabetes Research and Clinical Practice*, *183*, 109083. https://doi.org/10.1016/j.diabres.2021.109083

Pescitelli, G., Di Bari, L., & Berova, N. (2011). Conformational aspects in the studies of organic compounds by electronic circular dichroism. *Chemical Society Reviews*, *40*(9), 4603–4625. https://doi.org/10.1039/c1cs15036g

Pires, Blundell, T. L., & Ascher, D. B. (2015). pkCSM : predicting small-molecule pharmacokinetic properties using graph-based signatures (Theory- How to Enterpret pkCSM Result). *PKCSM*, 4. http://biosig.unimelb.edu.au/pkcsm/theory

Putri Dafriani, Mutiara Karamika, Siska Sakti Anggraini, & Roza Marlinda. (2020). The Potential of Noni (Moringa citrifolia) in Lowering Blood Glucose Levels in Diabetes Mellitus Patients. *Bioeduscience*, *4*(2), 120–123. https://doi.org/10.22236/j.bes/424919

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., Kesuma, D., & Siswandono. (2022a). Design, Molecular Docking, and Molecular Dynamics of thiourea-iron (III) metal Complexes as NUDT5 Inhibitors for Breast Cancer Treatment. *Heliyon*, *8*(9). https://doi.org/10.1016/j.heliyon.2022.e10694

Ruswanto, R., Nofianti, T., Mardianingrum, R., Kesuma, D., & Siswandono. (2022b). Design, Molecular Docking, And Molecular Dynamics Of Thiourea-Iron (III) Metal Complexes As NUDT5 Inhibitors For Breast Cancer Treatment. *Heliyon*, *8*(9). https://doi.org/10.1016/j.heliyon.2022.e10694

Sakulkeo, O., Wattanapiromsakul, C., Pitakbut, T., & Dej-Adisai, S. (2022). Alpha-Glucosidase Inhibition and Molecular Docking of Isolated Compounds from Traditional Thai Medicinal Plant, Neuropeltis Racemosa Wall. *Molecules*, *27*(3). https://doi.org/10.3390/molecules27030639

Salomon-Ferrer, R., Case, D. A., & Walker, R. C. (2013). An overview of the Amber biomolecular simulation package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, *3*(2), 198–210. https://doi.org/10.1002/wcms.1121

Sharma, V., Wakode, S., & Kumar, H. (2021). Structure- And Ligand-Based Drug Design: Concepts, Approaches, and Challenges. *Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences*, *January*, 27–53. https://doi.org/10.1016/B978-0-12-821748-1.00004-X

Siagian, J. I., Purnomo, H., & Sasmito, E. (2022). Studi In Silico Senyawa Dalam Teripang Sebagai Imunomodulator. *Journal of Pharmaceutical And Sciences*, *5*(1), 33–41. https://doi.org/10.36490/journal-jps.com.v5i1.99

Sina, H., Dramane, G., Tchekounou, P., Assogba, M. F., Chabi-Sika, K., Boya, B., Socohou, A., Adjanohoun, A., & Baba-Moussa, L. (2021). Phytochemical Composition and In Vitro Biological Activities of Morinda Citrifolia Fruit Juice. *Saudi Journal of Biological Sciences*, *28*(2), 1331–1335. https://doi.org/10.1016/j.sjbs.2020.11.059

Soelistijo, S. (2021). Pedoman Pengelolaan dan Pencegahan Diabetes Melitus Tipe 2 Dewasa di Indonesia 2021. *Global Initiative for Asthma*, 46. www.ginasthma.org.

Sovia, A. B., & Neva, M. (2017). Prediksi Mekanisme Kerja Obat Terhadap Reseptornya Secara In Silico(Studi Pada Antibiotika Sefotaksim). *Research Report*, *0*(0), 89–94. http://research-report.umm.ac.id/index.php/research-report/article/view/1367

Srivastava, N., Garg, P., Srivastava, P., & Seth, P. K. (2021). A molecular dynamics simulation study of the ACE2 receptor with screened natural inhibitors to identify novel drug candidate against COVID-19. *PeerJ*, *9*, 1–18. https://doi.org/10.7717/peerj.11171

Taghizadeh, M. S., Niazi, A., Moghadam, A., & Afsharifar, A. (2022). Experimental, molecular docking and molecular dynamic studies of natural products targeting overexpressed receptors in breast cancer. *PLoS ONE*, *17*(5

May), 1–14. https://doi.org/10.1371/journal.pone.0267961

Torres, M. A. O., de Fátima Braga Magalhães, I., Mondêgo-Oliveira, R., de Sá, J. C., Rocha, A. L., & Abreu-Silva, A. L. (2017). One Plant, Many Uses: A Review of The Pharmacological Applications of Morinda Citrifolia. *Phytotherapy Research*, *31*(7), 971–979. https://doi.org/10.1002/ptr.5817

Uciechowska-Kaczmarzyk, U., Chauvot de Beauchene, I., & Samsonov, S. A. (2019). Docking software performance in protein-glycosaminoglycan systems. *Journal of Molecular Graphics and Modelling*, *90*, 42–50. https://doi.org/10.1016/j.jmgm.2019.04.001

Weiss, R. (2019). Pathophysiology of Insulin Resistance and Type 2 Diabetes. In *Pediatric Type II Diabetes*. Elsevier Inc. https://doi.org/10.1016/B978-0-323-55138-0.00001-2

Weni, M., Safithri, M., & Seno, D. S. H. (2020). Molecular Docking of Active Compounds Piper crocatum on the A-Glucosidase Enzyme as Antidiabetic. *Indonesian Journal of Pharmaceutical Science and Technology*, *7*(2), 64. https://doi.org/10.24198/ijpst.v7i2.21120

Zafar, M., Khan, H., Rauf, A., Khan, A., & Lodhi, M. A. (2016). In Silico Study Of Alkaloids As α-Glucosidase Inhibitors: Hope For The Discovery Of Effective Lead Compounds. *Frontiers in Endocrinology*, *7*(DEC), 1–17. https://doi.org/10.3389/fendo.2016.00153

Zhu, Z. Y. (1995). A new approach to the evaluation of protein secondary structure predictions at the level of the elements of secondary structure. *Protein Engineering, Design and Selection*, *8*(2), 103–108. https://doi.org/10.1093/protein/8.2.103