DAFTAR PUSTAKA

Abdullah, S. S., Putra, P. P., Antasionasti, I., Rundengan, G., Suoth, E. J., Abdullah, R. P. I., & Abdullah, F. (2021). ANALISIS SIFAT FISIKOKIMIA, FARMAKOKINETIK DAN TOKSIKOLOGI PADA PERICARPIUM PALA (Myristica fragransa) SECARA ARTIFICIAL INTELLIGENCE. *Chemistry Progress*, *14*(2), 81. https://doi.org/10.35799/cp.14.2.2021.37112

Abraham, M. J., Murtola, T., Schulz, R., Páll, S., Smith, J. C., Hess, B., & Lindah, E. (2015). Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. *SoftwareX*, *1–2*, 19–25. https://doi.org/10.1016/j.softx.2015.06.001

Adeniji, S. E., Uba, S., & Uzairu, A. (2018). Theoretical modeling and molecular docking simulation for investigating and evaluating some active compounds as potent anti-tubercular agents against MTB CYP121 receptor. *Future Journal of Pharmaceutical Sciences*, *4*(2), 284–295. https://doi.org/10.1016/j.fjps.2018.10.003

Afriza, D., Suriyah, W. H., & Ichwan, S. J. A. (2018). In silico analysis of molecular interactions between the anti-apoptotic protein survivin and dentatin , nordentatin , and quercetin. *Journal of Physics: Conference Series*, *1073*(032001). https://doi.org/10.1088/1742-6596/1073/3/032001

Agu, P. C., Afiukwa, C. A., Orji, O. U., Ezeh, E. M., Ofoke, I. H., Ogbu, C. O., Ugwuja, E. I., & Aja, P. M. (2023). Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management. *Scientific Reports*, 1–18. https://doi.org/10.1038/s41598-023-40160-2

Al-karmalawy, A. A., Dahab, M. A., Metwaly, A. M., Elhady, S. S., Elkaeed, E. B., Eissa, I. H., & Darwish, K. M. (2021). *Molecular Docking and Dynamics Simulation Revealed the Potential Inhibitory Activity of ACEIs Against SARS-CoV-2 Targeting the h ACE2 Receptor*. *9*(May). https://doi.org/10.3389/fchem.2021.661230

Allouche, A. (2012). Software News and Updates Gabedit — A Graphical User Interface for Computational Chemistry Softwares. *Journal of Computational Chemistry*, *32*, 174–182. https://doi.org/10.1002/jcc

Amsad, L. N., Liliasari, L., Kadarohman, A., & Sardjono, R. E. (2023). *Connecting Students' Critical Thinking Skills with Conceptual Knowledge in Learning the Organic Compounds Stability by Using Marvin Sketch as a Tools to Adjust the Era of Society 5.0*. Atlantis Press SARL. https://doi.org/10.2991/978-2-38476-012-1_20

Arya, N., & Kaur, A. (2022). *Molecular Docking : A Review Paper*. *1*, 140–146.

Beshbishy, A., Wasef, L., Elewa, Y., Al-Sagan, A., Abd El-Hack, M., Taha, A., &

Abd-Elhakim, Y. (2020). Chemical Constituents and Pharmacological Activities of Garlic (Allium sativum L.): A Review. *Nutrients*, *12*(3), 872.

Boroujeni, M. B., Dastjerdeh, M. S., Shokrgozar, M., Rahimi, H., & Omidinia, E. (2021). Informatics in Medicine Unlocked Computational driven molecular dynamics simulation of keratinocyte growth factor behavior at different pH conditions. *Informatics in Medicine Unlocked*, *23*(February), 100514. https://doi.org/10.1016/j.imu.2021.100514

BPOM, Deputi Bidang Pengawasan Obat Tradisional, K. dan P. K., & Indonesia, D. O. A. (2014). *Bawang Putih (Allium Sativum L.)*.

Brogi, S., Ramalho, T. C., Kuca, K., Medina-Franco, J. L., & Valko, M. (2020). Editorial: In silico Methods for Drug Design and Discovery. *Frontiers in Chemistry*, *8*, 1–5. https://doi.org/10.3389/fchem.2020.00612

Burley, S. K., Berman, H. M., Christie, C., Duarte, J. M., Feng, Z., Westbrook, J., Young, J., & Zardecki, C. (2018). RCSB Protein Data Bank: Sustaining a living digital data resource that enables breakthroughs in scientific research and biomedical education. *Protein Science*, *27*(1), 316–330. https://doi.org/10.1002/pro.3331

Burley, S. K., Bhikadiya, C., Bi, C., Bittrich, S., Chao, H., Chen, L., Craig, P. A., Crichlow, G. V, Dalenberg, K., Duarte, J. M., Dutta, S., Fayazi, M., Feng, Z., Flatt, W., Ganesan, S., Ghosh, S., Goodsell, D. S., Green, K., Guranovic, V., … Zardecki, C. (2023). *RCSB Protein Data Bank (RCSB . org): delivery of experimentally-determined PDB structures alongside one million computed structure models of proteins from artificial intelligence / machine learning*. *51*(November 2022), 488–508.

Carugo, O., & Djinovic Carugo, K. (2013). Half a century of Ramachandran plots. *Acta Crystallographica Section D: Biological Crystallography*, *69*(8), 1333–1341. https://doi.org/10.1107/S090744491301158X

Castro-alvarez, A., Costa, A. M., & Vilarrasa, J. (2017). The Performance of Several Docking Programs at Reproducing Protein–Macrolide-Like Crystal Structures. *Molecules*, *22*(136). https://doi.org/10.3390/molecules22010136

Chaudhary, K. K., & Mishra, N. (2016). *A Review on Molecular Docking : Novel Tool for Drug Discovery*. *4*, 1–4.

Choudhary, S., Noor, M. U., & Hussain, M. S. (2022). Pharmacological properties and phytoconstituents of garlic (Allium sativum L.): A review. *Biological Sciences*, *02*(04). https://doi.org/10.55006/biolsciences.2022.2402

Chow, E., Rendleman, C. A., Bowers, K. J., Dror, R. O., Hughes, D. H., Gullingsrud, J., Sacerdoti, F. D., & Shaw, D. E. (2008). Desmond Performance on a Cluster of Multicore Processors Hardware and Operating Environment Benchmark Systems and Simulation Parameters. *DESRES/TR--2008-01 Desmond*, *1*, 1–14.

Colovos, C., & Yeates, T. O. (1993). Verification of protein structures: Patterns of nonbonded atomic interactions. *Protein Science*, *2*(9), 1511–1519. https://doi.org/10.1002/pro.5560020916

Dallakyan, S., & Olson, A. (2015). Participation in global governance: Coordinating "the voices of those most affected by food insecurity." *Global Food Security Governance*, *1263*, 1–11. https://doi.org/10.1007/978-1-4939-2269-7

Dutta, B., Banerjee, A., Chakraborty, P., & Bandopadhyay, R. (2018). In silico studies on bacterial xylanase enzyme: Structural and functional insight. *Journal of Genetic Engineering and Biotechnology*, *16*(2), 749–756. https://doi.org/10.1016/j.jgeb.2018.05.003

Elsliger, M. A., & Wilson, I. A. (2012). Structure validation and analysis. In *Comprehensive Biophysics* (Vol. 1). Elsevier Ltd. https://doi.org/10.1016/B978-0-12-374920-8.00110-7

Endriyanto, N. C., & Santoso, B. (2020). Hasil Komputasi Vina untuk Kandungan Bawang Putih dan Adas Bintang Terhadap Protein Dehidrogenase Piruvat Mycobacterium tuberculosis. *University Research Colloqium*, *1*(1), 366–372.

Fan, J., Fu, A., & Zhang, L. (2019). Progress in molecular docking. *Quantitative Biology*, *7*(2), 83–89. https://doi.org/10.1007/s40484-019-0172-y

Fantini, J., Devaux, C. A., Yahi, N., & Frutos, R. (2022). The novel hamster-adapted SARS-CoV-2 Delta variant may be selectively advantaged in humans. *Journal of Infection*, *84*(5), e53–e54. https://doi.org/10.1016/j.jinf.2022.03.001

Fiora Ladesvita, Ucip Sucipto, Ketut Lisnawati, Retno Dwi Santi, C. J. P. (2021). *Asuhan Keperawatan Onkologi Berdasarkan Teori Virginia Henderson*.

Friesner, R. A., Banks, J. L., Murphy, R. B., Halgren, T. A., Klicic, J. J., Mainz, D. T., Repasky, M. P., Knoll, E. H., Shelley, M., Perry, J. K., Shaw, D. E., Francis, P., & Shenkin, P. S. (2004). Glide: A New Approach for Rapid, Accurate Docking and Scoring. 1. Method and Assessment of Docking Accuracy. *Journal of Medicinal Chemistry*, *47*(7), 1739–1749. https://doi.org/10.1021/jm0306430

Globocan. (2020a). Cancer in Indonesia. *JAMA: The Journal of the American Medical Association*, *247*(22), 3087–3088. https://doi.org/10.1001/jama.247.22.3087

Globocan. (2020b). International Agency for Research on Cancer. *WHO Chronicle*, *23*(7), 323–326.

Gnesi, M., & Carugo, O. (2017). *How many water molecules are detected in X-ray protein crystal structures ? research papers*. 96–101. https://doi.org/10.1107/S1600576716018719

Goodsell, D. S., Dutta, S., Zardecki, C., Voigt, M., Berman, H. M., & Burley, S. K. (2015). The RCSB PDB "Molecule of the Month": Inspiring a Molecular View of Biology. *PLoS Biology*, *13*(5), 1–12. https://doi.org/10.1371/journal.pbio.1002140

Goodsell, D. S., Zardecki, C., Di Costanzo, L., Duarte, J. M., Hudson, B. P., Persikova, I., Segura, J., Shao, C., Voigt, M., Westbrook, J. D., Young, J. Y., & Burley, S. K. (2020). RCSB Protein Data Bank: Enabling biomedical research and drug discovery. *Protein Science*, *29*(1), 52–65. https://doi.org/10.1002/pro.3730

Gunasekaran, K., Ramakrishnan, C., & Balaram, P. (1996). Disallowed Ramachandran conformations of amino acid residues in protein structures. *Journal of Molecular Biology*, *264*(1), 191–198. https://doi.org/10.1006/jmbi.1996.0633

Haberkorn, U. (2019). What is cancer? *Advances in Nuclear Oncology:*, *62*(4), 1–16. https://doi.org/10.3109/9781420091380-2

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

Hevener, K. E., Zhao, W., Ball, D. M., Babaoglu, K., Qi, J., White, S. W., & Lee, R. E. (2009). Validation of Molecular Docking Programs for Virtual Screening against Dihydropteroate Synthase. *Journal of Chemical Information and Modeling*, *49*(2), 444–460. https://doi.org/10.1021/ci800293n

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

Hollingsworth, S. A., & Karplus, P. A. (2010). *A fresh look at the Ramachandran plot and the occurrence of standard structures in proteins*. *1*, 271–283. https://doi.org/10.1515/BMC.2010.022

Ivanovic, V., Rančić, M., Arsić, B., & Pavlović, A. (2020). Lipinski's rule of five, famous extensions and famous exceptions. *Chemia Naissensis*, *3*(1), 171–181. https://doi.org/10.46793/chemn3.1.171i

Jain, V., Kumar, H., Anod, H. V., Chand, P., Gupta, N. V., Dey, S., & Kesharwani, S. S. (2020). A review of nanotechnology-based approaches for breast cancer and triple-negative breast cancer. *Journal of Controlled Release*, *326*(July), 628–647. https://doi.org/10.1016/j.jconrel.2020.07.003

Jaydip, B., & Vraj, S. (2020). Identification of potent COVID-19 Main Protease (Mpro) inhibitors from Curcumin analogues by Molecular Docking Analysis. *International Journal of Advance Research, Ideas and Innovations in Technology*, *6*(2), 664–672.

Kadoura, A., Salama, A., & Sun, S. (2015). Switching Between the N V T and N pT Ensembles Using the Reweighting and Reconstruction Scheme. *Procedia - Procedia Computer Science*, *51*, 1259–1268. https://doi.org/10.1016/j.procs.2015.05.309

Kalibaeva, G., Ferrario, M., & Ciccotti, G. (2003). Constant pressure-constant temperature molecular dynamics : A correct constrained NPT ensemble using the molecular virial This article was downloaded by : On : 8 January 2011 Access details : Access Details : Free Access Constant pressure-constant tempera. *Molecular Physics*, *101*(6), 765–778. https://doi.org/10.1080/0026897021000044025

Khan, S. L., Sonwane, G. M., Siddiqui, F. A., Jain, S. P., Kale, M. A., & Borkar, V. S. (2020). *Discovery of Naturally Occurring Flavonoids as Human Cytochrome P450 (CYP3A4) Inhibitors with the Aid of Computational Chemistry*. *10*(4), 58–69.

Kim, N. B., Thuy, N. T., Minh, P. H., Thu, D. K., Tung, B. T., Kim, N. B., Thúy, N. T., & Hồ, P. (2021). *Screening Bioactive Compounds from Allium sativum as HER2 Inhibitors Targeting Breast Cancer by Docking Methods Sàng lọc các hợp chất ức chế thụ thể HER2 trong cây tỏi (Allium sativum) nhằm điều trị ung thư vú bằng phương pháp docking phân tử*. *37*(1), 35–47.

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. (2019). PubChem 2019 update: Improved access to chemical data. *Nucleic Acids Research*, *47*(D1), D1102–D1109. https://doi.org/10.1093/nar/gky1033

Kumar, A., & Zhang, K. Y. J. (2012). *Investigation on the E ff ect of Key Water Molecules on Docking Performance in CSARdock Exercise*.

Laskowski, R. A., Hutchinson, E. G., Michie, A. D., Wallace, A. C., Jones, M. L., & Thornton, J. M. (1997). PDBsum: A Web-based database of summaries and analyses of all PDB structures. *Trends in Biochemical Sciences*, *22*(12), 488–490. https://doi.org/10.1016/S0968-0004(97)01140-7

Laskowski, R. A., Jabłońska, J., Pravda, L., Vařeková, R. S., & Thornton, J. M. (2018). PDBsum: Structural summaries of PDB entries. *Protein Science*, *27*(1), 129–134. https://doi.org/10.1002/pro.3289

Lei, S., Zheng, R., Zhang, S., Wang, S., Chen, R., Sun, K., Zeng, H., Zhou, J., & Wei, W. (2021). Global patterns of breast cancer incidence and mortality: A population-based cancer registry data analysis from 2000 to 2020. *Cancer Communications*, *41*(11), 1183–1194. https://doi.org/10.1002/cac2.12207

Lewis-atwell, T., Townsend, P. A., & Grayson, M. N. (2022). *Comparing the Performances of Force Fields in Conformational Searching of Hydrogen-Bond-Donating Catalysts*. https://doi.org/10.1021/acs.joc.2c00066

Li, W., Zi-jun, W., Yi, L., Yong, W., & Rui-hua, D. I. (2008). *Design and*

Implementation of Parallel Lamarckian Genetic Algorithm for Automated Docking of Molecules. 689–694. https://doi.org/10.1109/HPCC.2008.50

Lionta, E., Spyrou, G., Vassilatis, D., & Cournia, Z. (2014). Structure-Based Virtual Screening for Drug Discovery: Principles, Applications and Recent Advances. *Current Topics in Medicinal Chemistry*, *14*(16), 1923–1938. https://doi.org/10.2174/1568026614666140929124445

Liu, X., Shi, D., Zhou, S., Liu, H., Liu, H., & Yao, X. (2018). Molecular dynamics simulations and novel drug discovery. *Expert Opinion on Drug Discovery*, *13*(1), 23–37. https://doi.org/10.1080/17460441.2018.1403419

Luethy, R. (2018). *VERIFY3D : Assessment of Protein Models with Three-Dimensional Profiles*. *6879*(April). https://doi.org/10.1016/S0076-6879(97)77022-8

Mahgoub, E. O., & Bolad, A. (2013). *Correctness and accuracy of template-based modeled single chain fragment variable (scFv) protein anti-breast cancer cell line (MCF-7)*. *2013*(September), 183–194.

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

Mazumder, L., Hasan, R., Fatema, K., & Islam, Z. (2022). *Structural and Functional Annotation and Molecular Docking Analysis of a Hypothetical Protein from Neisseria gonorrhoeae : An In-Silico Approach*. *2022*.

Miller, K. D., Nogueira, L., Devasia, T., Mariotto, A. B., Yabroff, K. R., Jemal, A., Kramer, J., & Siegel, R. L. (2022). Cancer treatment and survivorship statistics, 2022. *CA: A Cancer Journal for Clinicians*, *72*(5), 409–436. https://doi.org/10.3322/caac.21731

Mohanty, M., & Mohanty, P. S. (2023). Molecular docking in organic , inorganic , and hybrid systems : a tutorial review. *Monatshefte Für Chemie - Chemical Monthly*, *154*(7), 683–707. https://doi.org/10.1007/s00706-023-03076-1

Morris, G. M., Goodsell, D. S., Halliday, R. S., Huey, R., Hart, W. E., Belew, R. K., Olson, A. J., & Al, M. E. T. (1998). *Automated Docking Using a Lamarckian Genetic Algorithm and an Empirical Binding Free Energy Function*. *19*(14), 1639–1662.

Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S., & Olson, A. J. (2009). AutoDock4 and AutoDockTools4 : Automated Docking with Selective Receptor Flexibility. *Journal of Computational Chemistry*, *30*(16), 2785–2791. https://doi.org/10.1002/jcc

Muchtaridi, Arry Yanuar, Sandra Megantara, H. P. (2018). *Kimia Medisinal Dasar-Dasar Dalam Perancangan Obat*.

Muhammed, M. T., & Aki-yalcin, E. (1808). *Molecular Docking : Principles , Advances , and Its Applications in Drug Discovery*. 1–16. https://doi.org/10.2174/1570180819666220922103109

Muslikh, F. A., Dhafin, A. A., Prasetyawan, F., & Kadiri, U. (2023). *Prediction of Pinostrobin Pharmacokinetics from Temu Kunci (Boesenbergia rotunda (L .) Mansf .) Using pkCSM*. *1*(1), 1–6.

Muslikh, F. A., Kurniawati, E., Ma, B., Ilmu, I., Bhakti, K., Islam, U., Maulana, N., Brw, K. V, & Kadiri, U. (2023). *ADMET Prediction of the Dominant Compound from Mangosteen (Garcinia mangostana L .) using pkCSM : A Computational Approach*. *1*(1), 33–38.

Numan, M., Anwer, S., Id, B., Rehman, M.-, Mustafa, G., & Sadia, B. (2021). *Phylogenetic analyses , protein modeling and active site prediction of two pathogenesis related (PR2 and PR3) genes from bread wheat*. 1–16. https://doi.org/10.1371/journal.pone.0257392

Nurmik, M., Ullmann, P., Rodriguez, F., Haan, S., & Letellier, E. (2020). In search of definitions: Cancer-associated fibroblasts and their markers. *International Journal of Cancer*, *146*(4), 895–905. https://doi.org/10.1002/ijc.32193

Owoloye, A. J., Ligali, F. C., Enejoh, O. A., Musa, A. Z., Aina, O., Id, E. T. I., & Id, K. M. O. (2022). *Molecular docking , simulation and binding free energy analysis of small molecules as Pf HT1 inhibitors*. 1–18. https://doi.org/10.1371/journal.pone.0268269

Pinter, L. (1982). The new scaling table for the tonometer of Maklakov. *Szemeszet Ophthalmologica Hungarica*, *119*(2), 107–111.

Pinzi, L., & Rastelli, G. (2019). Molecular docking: Shifting paradigms in drug discovery. *International Journal of Molecular Sciences*, *20*(18). https://doi.org/10.3390/ijms20184331

Pires, D. E. V., Blundell, T. L., & Ascher, D. B. (2015). pkCSM: Predicting small-molecule pharmacokinetic and toxicity properties using graph-based signatures. *Journal of Medicinal Chemistry*, *58*(9), 4066–4072. https://doi.org/10.1021/acs.jmedchem.5b00104

Pratiwi, S. T. (2008). *Mikrobiologi Farmasi*.

Rachmania, R. A., Hariyanti, H., Zikriah, R., & Sultan, A. (2018). Studi In Silico Senyawa Alkaloid Herba Bakung Putih (Crinum Asiaticum L.) pada Penghambatan Enzim Siklooksigenase (COX). *Jurnal Kimia VALENSI*, *4*(2), 124–136. https://doi.org/10.15408/jkv.v4i2.7686

Ramirez, D., & Caballero, J. (2018). Is It Reliable to Take the Molecular Docking Top Scoring Position as the Best Solution without Considering Available Structural Data ? *Molecules*, *23*(1038), 1–17. https://doi.org/10.3390/molecules23051038

Reich, V., Majumdar, A., Müller, M., & Busch, S. (2022). Comparison of molecular dynamics simulations of water with neutron and X-ray scattering experiments. *EPJ Web of Conferences 272*, *01015*. https://doi.org/https://doi.org/10.1051/epjconf/202227201015

Renadi, S., Pratita, A. T. K., Mardianingrum, R., & Ruswanto, dan R. (2023). The Potency of Alkaloid Derivates as Anti-Breast Cancer Candidates: In Silico Study. *Jurnal Kimia Valensi*, *9*(1), 89–108. https://doi.org/10.15408/jkv.v9i1.31481

Richard, S. & M. W. H. (2014). *The Organic Chemistry of Drug Desigen and Drug Action*.

Rose, Y., Duarte, J. M., Lowe, R., Segura, J., Bi, C., Bhikadiya, C., Chen, L., Rose, A. S., Bittrich, S., Burley, S. K., & Westbrook, J. D. (2021). RCSB Protein Data Bank: Architectural Advances Towards Integrated Searching and Efficient Access to Macromolecular Structure Data from the PDB Archive. *Journal of Molecular Biology*, *433*(11), 166704. https://doi.org/10.1016/j.jmb.2020.11.003

Ruswanto, R. (2015). Molecular Docking Empat Turunan Isonicotinohydrazide Pada Mycobacterium Tuberculosis Enoyl-Acyl Carrier Protein Reductase (InhA). *Jurnal Kesehatan Bakti Tunas Husada: Jurnal Ilmu-Ilmu Keperawatan, Analis Kesehatan Dan Farmasi*, *13*(1), 135–141. https://doi.org/10.36465/jkbth.v13i1.25

Ruswanto, R., Mardianingrum, R., Nofianti, T., Fizriani, R., & Siswandono, S. (2023). Computational Study of Bis-(1-(Benzoyl)-3-Methyl Thiourea) Platinum (II) Complex Derivatives as Anticancer Candidates. *Advances and Applications in Bioinformatics and Chemistry*, *16*(January), 15–36. https://doi.org/10.2147/AABC.S392068

Ruswanto, R., Mardianingrum, R., Septian, A. D., & Yanuar, A. (2023). The design and virtual screening of thiourea derivatives as a Sirtuin-1 inhibitor. *Pharmacia*, *70*(4), 1335–1344. https://doi.org/10.3897/PHARMACIA.70.E108012

Ruswanto, R., Mardianingrum, R., Siswandono, S., & Kesuma, D. (2020). Reverse docking, molecular docking, absorption, distribution, and toxicity prediction of artemisinin as an anti-diabetic candidate. *Molekul*, *15*(2), 88–96. https://doi.org/10.20884/1.jm.2020.15.2.579

Ruswanto, R., Nofianti, T., Lestari, T., Septian, A. D., Firmansyah, A. P., & Mardianingrum, R. (2024). Potential Active Compounds of Propolis as Breast Anticancer Candidates: In Silico Study. *Jordan Journal of Biological Sciences*, *17*(1), 153–161. https://doi.org/10.54319/jjbs/170115

Ruswanto, R., Nofianti, T., Mardianingrum, R., Kesuma, D., & Siswandono. (2022). 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., & 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, Rahayuningsih, N., Hidayati, N. L. D., Nuryani, G. S., & Mardianingrum2, R. (2019). Uji In Vitro dan Studi In Silico Senyawa Turunan N ' -Benzoylisonicotinohydrazide sebagai Kandidat Antituberkulosis (In Vitro and In Silico Study of N ' -Benzoylisonicotinohydrazide as Antituberculosis Candidate). *Jurnal ILmu Kefarmasian Indonesia*, *17*(2), 218–226.

Saleem, H., Munir, S., Mumtaz, A., Ali, R., Maqbool, A., Malik, D., & Sideeq, M. A. (2019). Identification of Potent Inhibitors against Potential Drug Target for Schizophrenia Trough Virtual Screening Approach. *International Journal of Scientific and Research Publications (IJSRP)*, *9*(6), p90119. https://doi.org/10.29322/ijsrp.9.06.2019.p90119

Sanjaya, R. E., Putri, K. D. A., Kurniati, A., Rohman, A., & Puspaningsih, N. N. T. (2021). In silico characterization of the GH5-cellulase family from uncultured microorganisms: physicochemical and structural studies. *Journal of Genetic Engineering and Biotechnology*, *19*(1). https://doi.org/10.1186/s43141-021-00236-w

Sargsyan, K., Grauffel, C., & Lim, C. (2017). How Molecular Size Impacts RMSD Applications in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, *13*(1), 1518–1524. https://doi.org/10.1021/acs.jctc.7b00028

Senn, H. M., & Thiel, W. (2009). QM/MM methods for biomolecular systems. *Angewandte Chemie - International Edition*, *48*(7), 1198–1229. https://doi.org/10.1002/anie.200802019

Septian, A. D., Wardani, G. A., Mardianingrum, R., & Ruswanto, R. (2023). The Virtual Screening of Flavonoid Derivatives on Progesterone, Estrogen, and HER-2 Receptor for Breast Cancer Treatment Candidate. *Jurnal Kimia Valensi*, *9*(1), 163–182. https://doi.org/10.15408/jkv.v9i1.31482

Shaker, B., Ahmad, S., Lee, J., Jung, C., & Na, D. (2021). In silico methods and tools for drug discovery. *Computers in Biology and Medicine*, *137*(September), 104851. https://doi.org/10.1016/j.compbiomed.2021.104851

Shang, A., Cao, S. Y., Xu, X. Y., Gan, R. Y., Tang, G. Y., Corke, H., Mavumengwana, V., & Li, H. Bin. (2019). Bioactive compounds and biological functions of garlic (allium sativum L.). *Foods*, *8*(7), 1–31. https://doi.org/10.3390/foods8070246

Shivanika, C., Deepak Kumar, S., Ragunathan, V., Tiwari, P., Sumitha, A., & Brindha Devi, P. (2022). Molecular docking, validation, dynamics simulations, and pharmacokinetic prediction of natural compounds against the SARS-CoV-2 main-protease. *Journal of Biomolecular Structure and Dynamics*, *40*(2), 585–611. https://doi.org/10.1080/07391102.2020.1815584

Shofi, M. (2022). STUDI IN SILICO SENYAWA KUARSETIN DAUN KENCANA UNGU (Ruellia tuberosa L.) SEBAGAI AGEN ANTIKANKER PAYUDARA. *Jurnal Sintesis: Penelitian Sains, Terapan Dan Analisisnya*, *2*(1), 1–9. https://doi.org/10.56399/jst.v2i1.13

Singh, A., & Mishra, A. (2022). Molecular Dynamics Free Energy Simulation study to Investigate Binding Pattern of Isoliquiritigenin as PPAR ? Agonist. *PREPRINT (Version 1) Available at Research Square*, 1–20. https://doi.org/https://doi.org/10.21203/rs.3.rs-1046506/v1 License:

Srivastava, A., Malik, S., & Debnath, A. (2019). Heterogeneity in structure and dynamics of water near bilayers using TIP3P and TIP4P / 2005 water models. *Chemical Physics*, *525*(May), 110396. https://doi.org/10.1016/j.chemphys.2019.110396

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

Tam, B., Sinha, S., & Wang, S. M. (2020). Combining Ramachandran plot and molecular dynamics simulation for structural-based variant classification: Using TP53 variants as model. *Computational and Structural Biotechnology Journal*, *18*, 4033–4039. https://doi.org/10.1016/j.csbj.2020.11.041

Tao, X., Huang, Y., Wang, C., Chen, F., Yang, L., Ling, L., Che, Z., & Chen, X. (2020). Recent developments in molecular docking technology applied in food science: a review. *International Journal of Food Science and Technology*, *55*(1), 33–45. https://doi.org/10.1111/ijfs.14325

Tjitraresmi, A., Moektiwardoyo, M., Susilawati, Y., Megantara, S., Shiono, Y., & Ruswanto, R. (2022). THE VIRTUAL SCREENING OF SECONDARY METABOLITES OF MIANA LEAVES (Plectranthus scutellarioides (L) R. Br) AGAINST PLASMODIUM FALCIPARUM LACTATE DEHYDROGENASE ENZYME (PfLDH). *Rasayan Journal of Chemistry*, *15*(3), 2155–2164. https://doi.org/10.31788/RJC.2022.1536963

Tomasiak, L., Karch, R., & Schreiner, W. (2020). Long-Term Molecular Dynamics Simulations Reveal Flexibility Properties of a Free and TCR-Bound pMHC-I System. *2020 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*, 1295–1302. https://doi.org/10.1109/BIBM49941.2020.9313545

Torres, P. H. M., Sodero, A. C. R., Jofily, P., & Silva-Jr, F. P. (2019). Key topics in molecular docking for drug design. *International Journal of Molecular Sciences*, *20*(18), 1–29. https://doi.org/10.3390/ijms20184574

Wallner, B. (2006). Identification of correct regions in protein models using structural, alignment, and consensus information. *Protein Science*, *15*(4), 900–913. https://doi.org/10.1110/ps.051799606

Yeni, Y., & Rachmania, R. A. (2022). The Prediction of Pharmacokinetic Properties of Compounds in Hemigraphis alternata (Burm.F.) T. Ander Leaves Using pkCSM. *Indonesian Journal of Chemistry*, *22*(4), 1081–1089. https://doi.org/10.22146/ijc.73117

Yu, X. (2021). Prediction of inhibitory constants of compounds against SARS-CoV 3CLpro enzyme with 2D-QSAR model. *Journal of Saudi Chemical Society*, *25*(7), 101262. https://doi.org/10.1016/j.jscs.2021.101262

Yunita Sari, A., & Febrina, E. (2023). Potensi Senyawa Aktif Tanaman Herbal untuk Pengobatan Kanker Payudara dengan Metode Penambatan Molekuler: Review Artikel. *Jurnal Farmasi Udayana*, *12*(1), 23. https://doi.org/10.24843/jfu.2023.v12.i01.p04

Yunta, M. J. R. (2016). Docking and Ligand Binding Affinity : Uses and Pitfalls. *American Journal of Modeling and Optimization*, *4*(3), 74–114. https://doi.org/10.12691/ajmo-4-3-2

Zhou, A. Q., Hern, C. S. O., & Regan, L. (2011). *Revisiting the Ramachandran plot from a new angle*. *20*, 1166–1171. https://doi.org/10.1002/pro.644