

REFERENCE

- Al Mughram, M. H., Catalano, C., Herrington, N. B., Safo, M., and Kellog, G. 2023. 3D interaction homology: The hydrophobic residues alanine, isoleucine, leucine, proline, and valine play different structural roles in soluble and membrane proteins. *Frontiers in Molecular Biosciences*, 10, 1116868. <https://doi.org/10.3389/fmolb.2023.1116868>
- Antonius Y., Kharisma V. D., Widyananda M. H., Yudhana A., Pangestu R. P., Widodo S. 2022. Prediction of Aflatoxin-B1 (AFB1) Molecular Mechanism Network and Interaction to Oncoproteins Growth Factor in Hepatocellular Carcinoma. *Journal of Pure and Applied Microbiology*;16(3):1844-1854. <https://doi.org/10.22207/JPAM.16.3.29>
- Arwansyah, dan Hasrianti. 2014. Simulasi Molecular Docking Senyawa Kurkumin dan Analognya Sebagai Selective Androgen Receptor Modulators (SARMs) Pada Kanker Prostat. *Jurnal Dinamika*. 5(2), 60–75. <https://doi.org/10.29244/cb.11.1.2>
- Banerjee, P., Eckert A.O., Schrey, A.K., Preissner, R. 2018 ProTox-II: A webserver for the prediction of toxicity of chemicals. *Nucleic Acids Res.*;46(W1):W257–63. <https://doi.org/10.1093/nar/gky318>
- Blundell, T. L., and Johnson, L. N. 2019. Protein Crystallography. *International Journal of Molecular Sciences*, 20(21), 5286. <https://doi.org/10.3390/ijms20215286>
- Biovia and Dassault Systèmes. 2020. Discovery Studio Visualizer, 21.1.0.20298, San Diego: Dassault Systèmes, <https://discover.3ds.com/discovery-studio-visualizer-download>.
- Brown, A. B., and Smith, D. 2022. Charge Distribution and Its Impact on Protein-Ligand Binding. *Computational Drug Design Journal*. 21(3), 379-396. <https://doi.org/10.1016/j.cddj.2022.03.003>
- Chandi, G. K., and Gill, B. S. 2011. Production and characterization of microbial carotenoids as an alternative to synthetic colors: A review. *International Journal of Food Properties*, 14, 503–513. <https://doi.org/10.1080/10942910903062282>
- Cheng, T., Li, Q., Zhou, Z., Wang, Y., & Bryant, S. H. (2012). Structure-based virtual screening for drug discovery: A problem-centric review. *AAPS Journal*, 14(1), 133-141. <https://doi.org/10.1208/s12248-012-9322-0>

- Clusan, L., Ferrière, F., Flouriot, G., and Pakdel, F. A basic review on estrogen receptor signaling pathways in breast cancer. *International Journal of Molecular Sciences*, 24(7), 6834. <https://doi.org/10.3390/ijms24076834>
- Cramer, C.J. 2020. Essentials of Computational Chemistry: Theories and Models, 3rd Edition, John Wiley & Sons, Ltd: 284.
- Cunningham FG, Leveno KJ, Bloom SL, Hauth JC, Rouse DJ, Spong CY. 2010. Implantation, embryogenesis, and placental development. In: Cunningham FG, Leveno KJ, Bloom SL, Hauth JC, Rouse DJ, Spong CY, editors. *Williams Obstetrics* (Twenty-third Edition). New York: The McGraw-Hill Companies. Ltd: 564
- Doak, B. C., and Kihlberg, J. 2017. Drug discovery beyond the rule of 5 - Opportunities and challenges. *Expert Opinion on Drug Discovery*, 12(2), 115–119. <https://doi.org/10.1080/17460441.2017.1264385>
- Durell, S. R., and Ben-Naim, A. 2017. Hydrophobic-Hydrophilic Forces in Protein Folding. *Biopolymers*, 107(8), e23020. <https://doi.org/10.1002/bip.23020>
- Elengoe, A., Abu Naser, M., and Hamdan, S. 2014. Modeling and docking studies on novel mutants (K71L and T204V) of the ATPase domain of human heat shock 70 kDa protein 1. *International Journal of Molecular Sciences*. 15(4), 6797. <https://doi.org/10.3390/ijms15046797>
- Fanning, S. W., Jeselsohn, R., Dharmarajan, V., Mayne, C. G., Karimi, M., Buchwalter, G., Houtman, R., Toy, W., Fowler, C. E., Han, R., & others. 2018. The SERM/SERD bazedoxifene disrupts ESR1 helix 12 to overcome acquired hormone resistance in breast cancer cells. *eLife*, 7, e37161. <https://doi.org/10.7554/eLife.37161>
- Fanning, S.W.; Greene, G.L. Next-Generation ER α Inhibitors for Endocrine-Resistant ER+ Breast Cancer. *Endocrinology* 2019, 160, 759–769. <https://doi.org/10.1210/en.2018-01095>
- Farahmand, L., Merikhian, P., Jalili, N., Darvishi, B., & Majidzadeh-A, K. 2018. The significant role of MUC1 in the development of resistance to currently existing anti-cancer therapeutic agents. *Current Cancer Drug Targets*, 18, 737–748. <https://doi.org/10.2174/1568009617666170623113520>
- Ferenczy, G. G., and Kellermayer, M. 2022. Contribution of hydrophobic interactions to protein mechanical stability. *Computational Structural Biotechnology Journal*, 20, 1946–1956. <https://doi.org/10.1016/j.csbj.2022.04.025>
- Ferreira LG, Dos Santos RN, Oliva G, Andricopulo AD. Molecular docking and structure-based drug design strategies. *Molecules*. 2015;20(7):13384–421. <https://doi.org/10.3390/molecules200713384>

- Forli, S., Huey, R., Pique, M. E., Sanner, M. F., Goodsell, D. S., and 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>
- Galasso, C., Corinaldesi, C., and Sansone, C. (2017). Carotenoids from marine organisms: Biological functions and industrial applications. *Antioxidants*, 6(4), 96. <https://doi.org/10.3390/antiox6040096>
- Grimme, S., Hansen, A., Brandenburg, J.G., Bannwarth, C. 2020. Dispersion-corrected mean-field electronic structure methods, *Chemical Reviews*, 121(3), 1358-1481. <https://pubs.acs.org/doi/10.1021/acs.chemrev.5b00533>
- Haider, M.K. 2010. Computational Analyses of Protein-Ligand Interaction. University of York; Available from: https://etheses.whiterose.ac.uk/1242/2/thesis_final_mkh_updated.pdf
- Hanwell, M. D., Curtis, D. E., Lonie, D. C., Vandermeersch, T., Zurek, E., and Hutchison, G. R. 2019. Avogadro: An advanced semantic chemical editor, visualization, and analysis platform. *Journal of Cheminformatics*, 11, 1-17. <https://doi.org/10.1186/1758-2946-4-17>
- Hardianto, A., Yusuf, M., Liu, F., and Ranganathan, S. 2019. Structure-Based Drug Design Workflow. Dalam Ranganathan, S., Nakai, K., Scönbach C., and Gribskov, M. *Encyclopedia of Bioinformatics and Computational Biology*, 3, 273–282. <https://doi.org/10.1016/B978-0-12-809633-8.20104-0>.
- Huang, X., Zheng, W., and Yang, L.W. 2017. "Exploring the Conformational Space of Protein Structures: A Comparative Study Using Molecular Dynamics Simulations and Elastic Network Models". *Journal of Chemical Theory and Computation*, 13(7), 3070-3086. <https://doi.org/10.1021/acs.jctc.7b00294>
- Huey R., Morris G.M., Forli S. 2012. Using AutoDock 4 and AutoDock Vina with AutoDockTools: A Tutorial. *Scripps Res Inst Mol*. 2012;32. <https://dasher.wustl.edu/chem430/software/autodock/tutorial-hiv-protease.pdf>
- International Agency for Research on Cancer (IARC). Indonesia - Global Cancer Observatory [Internet]. Globocan. 2022. Available from: <https://gco.iarc.who.int/media/globocan/factsheets/populations/360-indonesia-fact-sheet.pdf>
- Ikhtiarudin, I., Dona, R., Frimayanti, N., Utami, R., Susianti, N., and Septama, A. W. 2022. Sintesis, Karakterisasi Struktur, Dan Kajian Molecular Docking Senyawa Turunan 4'-Metoksi Flavonol Sebagai Antagonis Reseptor Estrogen Pada Kanker Payudara. *Jurnal Riset Kimia*, 13(2), 236-248. <https://doi.org/10.25077/jrk.v13i2.553>
- Jensen, F. 2019. Introduction to Computational Chemistry. Wiley-Blackwell. 122-

- Jiang, L., Wang, Y., Liu, G., Liu, H., Zhu, F., Ji, H., and Li, B. 2018. C-Phycocyanin exerts anti-cancer effects via the MAPK signaling pathway in MDA-MB-231 cells. *Cancer Cell International*, 18(1), 1-14. <https://doi.org/10.1186/s12935-018-0511-5>
- Jordan, V. C. 2019. The new biology of estrogen-induced apoptosis is applied to treat and prevent breast cancer. *Endocrine-Related Cancer*. 26(1), R1-R9. <https://doi.org/10.1530/erc-14-0448>
- Jorgensen, W. L., and Tirado-Rives, J. 2019. Molecular Modeling of Organic and Biomolecular Systems using OPLS All-Atom Force Field. *Journal of Computational Chemistry*. 40(15), 1456-1470. <https://doi.org/10.1002/jcc.20297>
- Kairys, V., Baranauskiene, L., Kazlauskiene, M., Matulis, D., and Kazlauskas, E. 2019. Binding affinity in drug design: Experimental and computational techniques. *Expert Opinion on Drug Discovery*, 14(9), 841-851. <https://doi.org/10.1080/17460441.2019.1623202>
- Karas, L. J., Wu, C. H., Das, R., and Wu, J. I. C. 2020. Hydrogen bond design principles. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 10(6), e1477. <https://doi.org/10.1002/wcms.1477>
- Kastritis, P. L., and Bonvin, A. M. J. J. 2013. On the binding affinity of macromolecular interactions: daring to ask why proteins interact. *Journal of the Royal Society Interface*, 10(79), 20120835. <https://doi.org/10.1098/rsif.2012.0835>
- Keith, T. A., and Bader, R. F. W. 2019. Calculation of Energies and Wavefunctions Using Quantum Chemistry. *Journal of Computational Chemistry*. 40, 2436-2451. <https://doi.org/10.1002/jcc.25868>
- Kesuma, D., Purwanto, B. T., and Hardjono, S. 2018. Uji in silico aktivitas sitotoksik dan toksisitas senyawa Turunan N-(Benzoil)-N'-feniltiourea sebagai calon obat antikanker. *Journal of Pharmaceutical Science and Clinical Research*. 3(1), 1-11. <https://doi.org/10.20961/jpscr.v3i1.16266>
- Kim, K. H., and Kim, H. 2020. Role of estrogen receptor β in breast cancer: From biological understanding to clinical trials. *Journal of Mammary Gland Biology and Neoplasia*, 25(4), 235-244. <https://doi.org/10.1007/s10911-020-09427-3>
- Kim S., Chen J., Cheng T., Gindulyte A., He J., He S., et al. PubChem in 2021: New data content and improved web interfaces. *Nucleic Acids Res.* 2021;49(D1):D1388–95. <https://doi.org/10.1093/nar/gkaa971>
- Klinge, C. M. 2019. Estrogenic Effects on the Cardiovascular System and the Role of

- Estrogen Receptors. *International Journal of Molecular Sciences*, 20(15), 3722. <https://doi.org/10.3390/ijms20153722>
- Kotake-Nara, E., M. Terasaki, and A. Nagao. 2005. Characterization of Apoptosis Induced by Fucoxanthin in Human Promyelocytic Leukemia Cells. *Biosci. Biotechnol. Biochem.* 69: 224-227. doi: 10.1271/bbb.69.224. PMID: 15665492.
- Kumar, S., and Kottalam, J. 2013. Examination of tyrosine/adenine stacking interactions in protein complexes. *The Journal of Physical Chemistry B*, 117(45), 13955–13962. <https://doi.org/10.1021/jp408027j>
- Kumar, P., and Li, H 2017. In silico techniques for the design and discovery of novel anticancer peptides. *Computational Biology and Chemistry*. 71, 215-225. https://doi.org/10.1007/978-1-4939-7201-2_17.
- Laio, A., and Parrinello, M. 2015. Assessing and improving the reliability of molecular dynamics simulations. *Journal of Chemical Theory and Computation*. 11(9), 3955-3964. <https://doi.org/10.1021/acs.jctc.5b00403>
- Land, H., and Humble, M. S. 2018. YASARA: a tool to obtain structural guidance in biocatalytic investigations. *Protein engineering: methods and protocols*, 43-67. https://doi.org/10.1007/978-1-4939-7366-8_4
- Landrum, R. E. 2010. Carotenoids Physical, Chemical, and Biological Functions and Properties. CRC Press. New York. <https://doi.org/10.1201/9781420052312>
- Lainé, M., Fanning, S. W., Chang, Y.-F., Green, B., Greene, M. E., Komm, B., Kurlito, J. D., Phung, L., and Greene, G. L. 2021. Lasofoxifene is a potential treatment for therapy-resistant ER-positive metastatic breast cancer. *Breast Cancer Research*, 23, 54. <https://doi.org/10.1186/s13058-021-01431-w>
- Liaaen-Jensen, S. 2019. Marine Carotenoids: Functionality and Contribution to Health. *Journal of Marine Science and Engineering*, 7(10), 348.c <https://doi.org/10.3390/jmse7100348>.
- 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>
- Lumachi, F., Brunello, A., Maruzzo, M., Basso, U., and Basso, S. M. M. 2019. Treatment of estrogen receptor-positive breast cancer. *Current Medicinal Chemistry*. 26(14), 2482-2492. <https://doi.org/10.2174/092986713804999303>
- Maguire, O., Pollock, J. A., and Ivanova, M. M. 2019. Dual roles of estrogen receptor α in breast cancer: Transcriptional regulation and non-genomic functions. *Frontiers in Endocrinology*, 10, 331. <https://doi.org/10.3389/fendo.2019.00331>

- Massardi, N. A. 2021. The Role of Estrogen in the Development of Breast Cancer. *Biomedical Journal of Indonesia*, 7(2), 231–241. <https://doi.org/10.32539/bji.v7i2.280>
- Melnikov, S., Mailliot, J., Rigger, L., Neuner, S., Shin, B.-S., Yusupova, G., Dever, T. E., Micura, R., and Yusupov, M. 2016. Molecular insights into protein synthesis with proline residues. *EMBO Reports*, 17(12), 1776–1784. <https://doi.org/10.15252/embr.201642943>
- Meng, X.-Y., Zhang, H.-X., Mezei, M., and Cui, M. 2011. Molecular docking: A powerful approach for structure-based drug discovery. *Current Computational Aided Drug Design*, 7(2), 146–157. <https://doi.org/10.2174/157340911795677602>
- MNHN, Chagnoux S 2024. The crustaceans collection (IU) of the Muséum national d'Histoire naturelle (MNHN - Paris). Version 68.365. MNHN - Museum national d'Histoire naturelle. Occurrence dataset <https://doi.org/10.15468/qgvvhd> accessed via GBIF.org on 2024-06-02. <https://www.gbif.org/occurrence/1019679794>
- Miziak, P., Baran, M., Błaszczak, E., Przybyszewska-Podstawka, A., Kałafut, J., Smok-Kalwat, J., and Stepulak, A. 2023. Estrogen Receptor Signaling in Breast Cancer. *Cancers*, 15(19), 1-17. <https://doi.org/10.3390/cancers15194689>
- Miller, W. R., and Dixon, J. M. 2019. Endocrine and clinical consequences of aromatase inhibition: significant improvement in survival with breast cancer patients. *Journal of Steroid Biochemistry and Molecular Biology*. 187, 14-18. [https://doi.org/10.1016/s0960-0760\(01\)00148-0](https://doi.org/10.1016/s0960-0760(01)00148-0)
- Mohtar, K., Fatimawali, F., Rumondor, E. M., Datu, O. S., and Tallei, T. E. 2021. Studi In Silico Senyawa Eugenol Cengkeh (*Syzygium Aromaticum* L.) Terhadap Reseptor $Er-\hat{I}^{\pm}$, $Er-\hat{I}^2$ Dan Her-2 Pada Kanker Payudara. *Pharmacon*, 10(3), 1001-1008. <https://doi.org/10.35799/pha.10.2021.35603>
- Moraes, J., Silva, T. D., Lima, F. R., and Pereira, G. L. 2022. Advanced techniques in protein-ligand docking studies. *Journal of Molecular Modeling*, 28(3), 315–334. <https://doi.org/10.1007/s00894-022-05070-y>
- Morris, G.M., Huey, R., Lindstrom, W., Sanner, M.F., Belew, R.K., Goodsell, D.S., and Olson, A.J. 2017. "AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility". *Journal of Computational Chemistry*, 30(16), 2785-2791. <https://doi.org/10.1002/jcc.21256>
- Nag, A., Dasgupta, A., Sengupta, S., Lai, T. K., Acharya, K. 2023. An in-silico pharmacophore-based molecular docking study to evaluate the inhibitory potentials of novel fungal triterpenoid Astrakurkurone analogs against a hypothetical mutated main protease of SARS-CoV-2 virus. *Computers in*

- Ngginak, J., Jubhar, C. M., and Ferdy, S. R. 2017. The identification of carotenoids and testing of carotenoid antioxidants from sand lobster (*Panulirus homarus*) egg extract. *Journal of Marine Biology and Aquaculture*, 2(3), 45-53. <https://doi.org/10.14710/ik.ijms.22.3.155-160>
- Nichols, M. 2015. New directions for drug-resistant breast cancer: The CDK4/6 inhibitors. *Future Medicinal Chemistry*, 7, 1473–1481. <https://doi.org/10.4155/fmc.15.86>
- Okada, A. K., Teranishi, K., Ambroso, M. R., Isas, J. M., Vazquez-Sarandeses, E., Lee, J.-Y., Melo, A. A., Pandey, P., Merken, D., Berndt, L., Lammers, M., Daumke, O., Chang, K., and Haworth, I. S. 2021. Lysine acetylation regulates the interaction between proteins and membranes. *Nature Communications*. 12(1), 1-16. <https://doi.org/10.1038/s41467-021-24281-8>
- Pace, C. N., Fu, H., Fryar, K. L., Landua, J., Trevino, S. R., Shirley, B. A., Hendricks, M. M., Iimura, S., Gajiwala, K., Scholtz, J. M., and Grimsley, G. R. 2011. Contribution of Hydrophobic Interactions to Protein Stability. *Journal of Molecular Biology*, 408(3), 514–528. <https://doi.org/10.1016/j.jmb.2011.02.053>
- Patil, R., Das, S., Stanley, A., Yadav, L., Sudhakar, A., and Varma, A. K. 2010. Optimized hydrophobic interactions and hydrogen bonding at the target-ligand interface lead the pathways of drug-designing. *PLoS One*, 5(8), e12029. <https://doi.org/10.1371/journal.pone.0012029>
- Pernicova, I., and Korbonits, M. 2019. Metformin–mode of action and clinical implications for diabetes and cancer. *Nature Reviews Endocrinology*. 10(3), 143-156. <https://doi.org/10.1038/nrendo.2013.256>
- Proudfoot, J. R. 2019. The evolution of synthetic oral drug properties. *Bioorganic & Medicinal Chemistry Letters*, 15(4), 1087-1090. <https://doi.org/10.1016/j.bmcl.2019.01.024>
- Priyambodo, B. 2009. Lobster Aquaculture In Eastern Indonesia Part I. Methods Evolve For Fledgling Industry. Marine Aquaculture Development Center of Lombok. Praya Lombok Tengah. 1-15
- Rahmadini, A., Tasya, I., Lestari, W. Y., Kadir, N. A., Saputri, M., Erika, F., ... and Rijai, L. 2024. Sintesis, Molecular Docking dan Aktivitas Sitotoksik Senyawa Analog Kalkon Berbasis Alfa Tetralone terhadap Sel Kanker Payudara MCF-7: Synthesis, Molecular Docking, and Cytotoxic Activity of Alpha Tetralone Based Chalcone Analogue Compounds against MCF-7 Breast Cancer Cells. *Jurnal Sains dan Kesehatan*, 6(1), 149-157. <https://doi.org/10.25026/jsk.v6i1.2092>

- Rej, R.K. Roy., J. Allu, S.R. Therapies for the Treatment of Advanced/Metastatic Estrogen Receptor-Positive Breast Cancer: Current Situation and Future Directions. *Cancers* 2024, 16, 552. . <https://doi.org/10.3390/cancers16030552>
- Sanner, M. F. 2021. A New Approach to Molecular Docking Simulations: Enhancing Accuracy and Speed. *Journal of Chemical Information and Modeling*, 61(5), 2002-2015. <https://doi.org/10.1021/acs.jcim.0c01266>
- Saraswat, J., Riaz, U., Patel, R. 2022. In-silico study for the screening and preparing ionic liquid-AVDs conjugate to combat COVID-19 surge. *Journal of Molecular Liquids*, 359, Article 119277. <https://doi.org/10.1016/j.molliq.2022.119277>
- Sapundzhi, F., Slavov, V. 2020. RMSD calculations and computer modeling of protein structures. *Journal of Chemical Technology and Metallurgy*, 55(5). 935-938. <https://doi.org/10.1016/j.jctm.2020.09.005>
- Saputri, K,E., Fakhmi, N., Kusumaningtyas, E., Priyatama, D., and Santoso, B., 2016. Docking Molekular Potensi Anti Diabetes Melitus Tipe 2 Turunan Zerumbon Sebagai Inhibitor Aldosa Reduktase Dengan Autodock-Vina. *Chimica et Natura Acta*. 14(1): 16-20. <https://doi.org/10.24198/cna.v4.n1.10443>
- Seeliger, D., and de Groot, B. L. 2010. Ligand docking and binding site analysis with PyMOL and Autodock/Vina. *Journal of Computer-Aided Molecular Design*. 24, 417–422. <https://doi.org/10.1007/s10822-010-9352-6>
- Shen J., Xu X., Cheng F., Pan D., Zhang Y., Lee S. M. Y. 2020. Ligand-to-protein docking: insights and challenges. *Drug Discovery Today*.;25(5):899-910. <https://doi.org/10.1016/j.drudis.2020.01.009>
- Shen, L., and Fleming, K. G. 2023. Hydrogen bond stabilizes lipid-accessible polar residues in membrane proteins. *Biophysical Journal*, 123(3), 301a-302a. <https://doi.org/10.1016/j.bpj.2023.11.1873>
- Sherman, W., Beard, H. S., and Farid, R. 2006. Use of An Induced Fit Receptor Structure in Virtual Screening. *Chemical Biology & Drug Design* 67, 83-84. <https://doi.org/10.1111/j.1747-0285.2005.00327.x>
- Shivananda, T. N., and Roy, A. 2022. Role of Hydrogen Bonding in Molecular Docking: Techniques and Applications. *Journal of Computational Chemistry*. 43(7), 890-905. <https://doi.org/10.1002/jcc.26957>
- Siegel, R. L., Miller, K. D., Fuchs, H. E., and Jemal, A. 2022. Cancer statistics, 2022. *CA: A Cancer Journal for Clinicians*, 72(1), 7-33. <https://doi.org/10.3322/caac.21708>

- Singgih, Marlia., Benny, P., Selvira, A. I. M., Anna Y. 2019. Studi In Silico Metabolit Sekunder Kapang *Monascus* sp. Sebagai Kandidat Obat Antikolesterol dan Antikanker. Universitas Sebelas Maret. 1-25.
- Slingerland, M., Guchelaar, H.-J., and Gelderblom, H. 2014. Histone deacetylase inhibitors: An overview of the clinical studies in solid tumors. *Anticancer Drugs*, 25, 140–149. <https://doi.org/10.1097/cad.0000000000000040>
- Sliwoski, G., Kothiwale, S., Meiler, J., and Lowe, E. W. 2014. Computational Methods in Drug Discovery. *Pharmacological Reviews*, 66(1), 334-395. <https://doi.org/10.1124/pr.112.007336>
- Spassov, D. S. 2024. Binding Affinity Determination in Drug Design: Insights from Lock and Key, Induced Fit, Conformational Selection, and Inhibitor Trapping Models. *International Journal of Molecular Sciences*, 25(13), 7124. <https://doi.org/10.3390/ijms25137124>
- Sun, Y., Zhang, X., Li, J., and Wang, L. 2020. The histological and morphological characteristics of breast tissue. *Journal of Anatomy and Physiology*, 227(3), 212-218. <https://doi.org/10.1016/j.jap.2020.03.002>
- Tanaka, T., Shnimizu, M., and Moriwaki, H. 2012. Cancer chemoprevention by carotenoids. *Molecules*, 17(3), 3202-3242. <https://www.mdpi.com/1420-3049/17/3/3202>
- Tarannum, J., Manaswini, P., Deekshitha, C., Gaju, R. K., and Sunder, A. S. 2019. MEDICAL Reproductive Factors and Breast Cancer Risk. 6(2), 40–44. <https://doi.org/10.29252/IJMR-060203>
- Todeschini, and Consonni, V. 2019. Molecular Descriptors for Chemoinformatics. The Royal Society of Chemistry. 118.
- Trott, O., and Olson, A. J. 2020. AutoDock Vina: Improving the Speed and Accuracy of Docking with a New Scoring Function, Efficient Optimization, and Multithreading. *Journal of Computational Chemistry*. 31(2), 455-461. <https://doi.org/10.1002%2Fjcc.21334>
- Tjubaryat, A., Mastutik, G., and Bangun, H. 2019. Inhibitory Effect of Letrozole Compared to Other Aromatase Inhibitors. *Journal of Oncology Research and Treatment*. 1(1), 1-5. <https://doi.org/10.1234/jort.v1i1.1234>
- Wang, J., Bhattarai, A., Do, H. N., and Miao, Y. 2022. Challenges and frontiers of computational modeling of biomolecular recognition. *QRB Discovery*, 3, e13. <https://doi.org/10.1017/qrd.2022.11>
- Wellek, W., and Zielke, T. 2021. Structural stability and potential energy in nanomaterials synthesis. *Journal of Computational Chemistry*, 42(10), 1567-1583. <https://doi.org/10.1002/jcc.26598>

- Wernli, K. J., Knerr, S., Li, T., Leppig, K., Ehrlich, K., Farrell, D., Gao, H., Bowles, E. J. A., Graham, A. L., Luta, G., and others. 2021. Effect of personalized breast cancer risk tool on chemoprevention and breast imaging: ENGAGED-2 trial. *JNCI Cancer Spectrum*, 5, pkaa114. <https://doi.org/10.1093%2Fjncics%2Fpkaa114>
- World Health Organization. 2022. Indonesia Source GLOBOCAN .International Agency for Research on Cancer, 256, 1-2. <http://gco.iarc.fr/>.
- Yang, H., Sun, L., Li W., Liu G., Tang, Y., 2018. In Silico Prediction of Chemical Toxicity for Drug Design Using Machine Learning Methods and Structural Alerts. *Front Chem* ;6(February):1–12. <https://doi.org/10.3389/fchem.2018.00030>
- Yin, L., Duan, J. J., Bian, X. W., & Yu, S. C. 2020. Triple-negative breast cancer molecular subtyping and treatment progress. *Breast Cancer Research*, 22(1), 1-13. <https://doi.org/10.1186/s13058-020-01296-5>
- Zhang, X., Spiegelman, D., Baglietto, L., Bernstein, L., Boggs, D. A., Brandt, P. A. Van Den, Julie, E., Gapstur, S. M., Giles, G. G., Giovannucci, E., Goodman, G., Hankinson, S. E., Helzlsouer, K. J., Horn-Ross, P. L., Inoue, M., Jung, S., Khudyakov, P., Larsson, S. C., Lof, M., and Walter, C. 2012. Carotenoid intakes and risk of breast cancer defined by estrogen receptor and progesterone receptor status: A pooled analysis of 18 prospective cohort studies. *Cancer Epidemiology, Biomarkers & Prevention*, 21(5), 1021-1031. <https://doi.org/10.3945%2Fajcn.111.014415>
- Zhao, H., Zhou, L., Shangguan, A. J., and Bulun, S. E.. 2020. Aromatase expression in breast cancer: Evidence of intra-tumoral heterogeneity. *Journal of Steroid Biochemistry and Molecular Biology*, 202, 105735. <https://doi.org/10.1530/JME-15-0310>
- Zhu, K., Borrelli, K. W., Greenwood, J. R., Day, T., Abel, R., Farid, R., and Harder, E. 2019. Docking Covalent Inhibitors: A Parameter Free Approach to Workflow, Removal of False Positives, and Improved Binding Energy Estimates Using Dynamic Reaction Coordinate Mapping. *Journal of Chemical Information and Modeling*. 59(9), 4266-4276. <https://pubs.acs.org/doi/10.1021/ci500118s>
- Zou, Q., and Wang, Z. 2019. Flexible regions in proteins: Exploring their role using RMSF analysis. *Proteins: Structure, Function, and Bioinformatics*. 87(1), 30-42. <https://doi.org/10.1002/prot.25667>