# DAFTAR PUSTAKA


Afzal, M., Alharbi, K. S., Kazmi, I., et al. (2022). *Green Tea Catechins Attenuate Neurodegenerative Diseases and Cognitive Deficits.* Molecules, 27(21), 7604. https://doi.org/10.3390/molecules27217604

Azmal, M., Hossen, M. S., Shohan, N. H., Taqui, R., Malik, A., & Ghosh, A. (2024). A computational approach to identify phytochemicals as potential inhibitor of acetylcholinesterase: Molecular docking, ADME profiling and molecular dynamics simulations. *PLOS ONE, 19*(6), e0304490. https://doi.org/10.1371/journal.pone.0304490

Baroroh, U., Muscifa, Z. S., Destiarani, W., Rohmatullah, F. G., & Yusuf, M. (2023). Molecular interaction analysis and visualization of protein-ligand docking using Biovia Discovery Studio Visualizer. *Indonesian Journal of Computational Biology (IJCB), 2*(1), 22. https://doi.org/10.24198/ijcb.v2i1.46322

Birks, J., & Harvey, R. J. (2018). *Donepezil for dementia due to Alzheimer's disease*. *Cochrane Database of Systematic Reviews*, (6), CD001190. https://doi.org/10.1002/14651858.CD001190.pub3

Bitencourt-Ferreira, G., & de Azevedo, W. F. (2019). *Docking Screens for Drug Discovery*. Cham: Springer Nature Switzerland AG. https://doi.org/10.1007/978-1-4939-9752-7

Bitencourt-Ferreira, G., Veit-Acosta, M., & de Azevedo, W. F. (2019). Van der Waals potential in protein complexes. *Methods in Molecular Biology, 2053*, 79–91. https://doi.org/10.1007/978-1-4939-9752-7_6

Bitew, M., Desalegn, T., & Demissie, T. B. (2021). In silico drug-likeness and ADMET prediction of phytochemicals. *Advances and Applications in Bioinformatics and Chemistry*, 14, 11–24.

Budryn, G., Majak, I., Grzelczyk, J., Szwajgier, D., Rodríguez-Martínez, A., & Pérez-Sánchez, H. (2022). Hydroxybenzoic acids as acetylcholinesterase inhibitors: Calorimetric and docking simulation studies. *Nutrients, 14*(12), 2476. https://doi.org/10.3390/nu14122476

Bulusu, G., & Desiraju, G. R. (2020). Strong and weak hydrogen bonds in protein–ligand recognition. *Journal of the Indian Institute of Science, 100*(1), 31–41. https://doi.org/10.1007/s41745-019-00141-9

Elfiky, A. A. (2021). Natural products may interfere with SARS-CoV-2 attachment to the host cell. *Journal of Biomolecular Structure and Dynamics, 39*(9), 3194–3203. https://doi.org/10.1080/07391102.2020.1761881

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

Fadhilah, Z. H., Perdana, F., Aldizal, R., & Rizkio, M. (2021). Review: Telaah kandungan senyawa katekin dan epigalokatekin galat (EGCG) sebagai antioksidan pada berbagai jenis teh. *Jurnal Pharmascience, 8*(1), 31–44.

Fadli, F., Patoding, S., & Asmar, A. (2023). *Pengaruh Terapi Brain Gym terhadap Peningkatan Fungsi Kognitif pada Lansia yang Menderita Demensia*. Jurnal Media Keperawatan: Politeknik Kesehatan Makassar, 14(2). E-ISSN 2622-0148, p-ISSN 2087-0035.

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

Farhah, A., Az-Zahra, F., Afidika, J., Diamantha, S. D. A., Rahmani, A. E., Fatimah, S., Aulifa, D. L., Elaine, A. A., & Sitinjak, B. D. P. (2022). *In Silico Study of Betel Leaves Compound (Piper betle L.) as Acetylcholinesterase (AchE) Enzyme Inhibitor in Alzheimer Disease.* Indonesian Journal of Biological Pharmacy, 2(2), 44–58.

Farina, N., Jacobs, R., Turana, Y., Fitri, F. I., Schneider, M., Theresia, I., Docrat, S., Sani, T. P., Augustina, L., Albanese, E., Comas-Herrera, A., Du Toit, P., Ferri, C. P., Govia, I., Ibnidris, A., Knapp, M., & Banerjee, S. (2023). Comprehensive measurement of the prevalence of dementia in low- and middle-income countries: STRiDE methodology and its application in Indonesia and South Africa. *BJPsych Open, 9*(e102). https://doi.org/10.1192/bjo.2023.76

Farkhondeh, T., Samarghandian, S., Azimi-Nezhad, M., & Samini, F. (2020). The neuroprotective effects of epigallocatechin-3-gallate (EGCG) in neurodegenerative diseases: A review. *European Journal of Pharmacology*, 889, 173596. https://doi.org/10.1016/j.ejphar.2020.173596

Feng, Z., Westbrook, J. D., Sala, R., Smart, O. S., Bricogne, G., Matsubara, M., Yamada, I., Tsuchiya, S., Aoki-Kinoshita, K. F., Hoch, J. C., Kurisu, G., Velankar, S., Burley, S. K., & Young, J. Y. (2021). Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. Structure, 29(4), 393-400.e1. https://doi.org/10.1016/j.str.2021.02.004

Girame, H., Garcia-Borràs, M., & Feixas, F. (2022). Changes in protonation states of in-pathway residues can alter ligand binding pathways obtained from spontaneous binding molecular dynamics simulations. *Frontiers in Molecular Biosciences, 9*, 922361. https://doi.org/10.3389/fmolb.2022.922361

Hollingsworth, S. A., & Dror, R. O. (2018). Review Molecular Dynamics Simulation for All. Neuron, 99(6), 1129–1143. https://doi.org/10.1016/j.neuron.2018.08.011

Islam, M. S., et al. (2024). *Combating multidrug-resistant bacterial infections through computational identification of Celecoxib and thymol derivatives targeting AcrB efflux pump*. Frontiers in Chemistry, 12. https://doi.org/10.3389/fchem.2024.1376783

Ivanović, M., Alimpić Aradski, A., & Šegan, S. (2020). Prediction of lipophilicity and pharmacokinetic properties of selected bioactive compounds. *Molecules, 25*(24), 5870. https://doi.org/10.3390/molecules25245870

Jaydip, B, dan Vraj, S. (2020). Identifikasi of Potent COVID-19 Main Protease (Mpro) Inhibitors from Curcumin Analogues by Molecular Docking Analysis. International Journal of Advance Research, 6(2), 664-672.

Kar, S., & Leszczynski, J. (2020). Exploration of computational approaches to predict ADMET properties of chemical compounds. *Current Topics in Medicinal Chemistry, 20*(20), 1809–1825. https://doi.org/10.2174/1568026620666200427163951

Kementerian Kesehatan Republik Indonesia. (2023). *Profil kesehatan Indonesia tahun 2022*. Kementerian Kesehatan Republik Indonesia.

Khan, M. T., et al. (2021). *Marine natural compounds as potents inhibitors against the main protease of SARS-CoV-2—A molecular dynamic study*. Journal of Biomolecular Structure and Dynamics. https://doi.org/10.1080/07391102.2020.1769733.

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, 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, 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

Li, S., Wang, Z., Liu, G., & Chen, M. (2024). Neurodegenerative diseases and catechins: (−)-epigallocatechin-3-gallate is a modulator of chronic neuroinflammation and oxidative stress. *Frontiers in Nutrition, 11*, 1425839. https://doi.org/10.3389/fnut.2024.1425839

Li, X., Feng, X., Sun, X., Hou, N., Han, F., & Liu, Y. (2022). Global, regional, and national burden of Alzheimer's disease and other dementias, 1990–2019. *Frontiers in Aging Neuroscience, 14*, 937486. https://doi.org/10.3389/fnagi.2022.937486

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

Maitsa, A. F., Banowati, N. D., Nurjanah, Y., Nurulaini, S. N., Athaya, S., Muchtaridi, M., Rusdin, A., & Mardisanutol, H. T. (2023). *In Silico Study of Black Pepper (Piper nigrum L.) Bioactive Compounds as Acetylcholinesterase (AchE) Enzyme Inhibitors in Alzheimer's Disease.* Indonesian Journal of Biological Pharmacy, 3(2), 106–119.

Malik, A., Taqui, R., Shohan, N. H., Hossen, M. S., Rahman, M. A., & Ghosh, A. (2022). Molecular docking and dynamic simulation study of phytocompounds

from medicinal plants as acetylcholinesterase inhibitors for Alzheimer's disease therapy. *Journal of Biomolecular Structure and Dynamics*. https://doi.org/10.1080/07391102.2022.2126548

Mansoori, R., Jain, D., Pandey, V., & Jain, S. K. (2022). *A comprehensive review on biological activity of green tea (Camellia sinensis).* Journal of Drug Delivery & Therapeutics, 12(5), 250–265. https://jddtonline.info/index.php/jddt/article/view/5613

Mazumder, L., Hasan, M. R., Fatema, K., Islam, M. Z., & Tamanna, S. K. (2022). *Structural and Functional Annotation and Molecular Docking Analysis of a Hypothetical Protein from Neisseria gonorrhoeae: An In-Silico Approach*. BioMed Research International, 2022, 1–12. https://doi.org/10.1155/2022/4302625.

Meli, R., & Biggin, P. C. (2020). *spyrmsd: Symmetry-corrected RMSD calculations in Python*. *Journal of Cheminformatics, 12*(1), 49. https://doi.org/10.1186/s13321-020-00455-2

Melo, K. R. T., Gomes, A. F., Silva, J. R. A., Oliveira, T. S., Lima, M. C. A., & Rolim, L. A. (2022). Molecular docking and dynamics simulation of natural compounds as acetylcholinesterase inhibitors for Alzheimer's disease treatment. *Journal of Biomolecular Structure and Dynamics, 40*(18), 8742–8755. https://doi.org/10.1080/07391102.2021.1932154

Mishra, G., Awasthi, R., Singh, A. K., Singh, S., Mishra, S. K., Nandi, M. K., & Tiwari, A. K. (2024). *Development of epigallocatechin and ascorbic acid dual delivery transferosomes for managing Alzheimer's disease: In vitro and in vivo studies*. ACS Omega, 9, 35463–35474. https://doi.org/10.1021/acsomega.4c02140

Mishra, S., Singh, P., & Kumari, K. (2022). Molecular docking and molecular dynamics simulation in drug discovery and development. *Frontiers in Molecular Biosciences, 9*, 828221. https://doi.org/10.3389/fmolb.2022.828221

Mokra, D., Joskova, M., & Mokry, J. (2022). Therapeutic effects of green tea polyphenol (−)-epigallocatechin-3-gallate (EGCG) in relation to molecular pathways controlling inflammation, oxidative stress, and apoptosis. *International Journal of Molecular Sciences, 24*(1), 340. https://doi.org/10.3390/ijms24010340

Nguyen, V. T. T., Sallbach, J., dos Santos Guilherme, M., & Endres, K. (2021). *Influence of acetylcholine esterase inhibitors and memantine, clinically approved for Alzheimer's dementia treatment, on intestinal properties of the mouse. International Journal of Molecular Sciences, 22*(3), 1015. https://doi.org/10.3390/ijms22031015

Nusantoro, Y. R., & Fadlan, A. (2021). *The Effect of Energy Minimization On The Molecular Docking of Acetone-Based Oxindale*. *6*(1), 69–77.

Okello, E. J., & Mather, J. (2020). Comparative kinetics of acetyl- and butyryl-cholinesterase inhibition by green tea catechins: Relevance to the symptomatic treatment of Alzheimer's disease. *Nutrients, 12*(4), 1090. https://doi.org/10.3390/nu12041090

Pantsar, T., & Poso, A. (2018). Binding affinity via docking: Fact and fiction. *Molecules, 23*(8), 1899. https://doi.org/10.3390/molecules23081899

Paramita, N. L. P. V., Andari, N. P. T. W., Andani, N. M. D., & Susanti, N. M. P. (2020). Penetapan kadar fenol total dan katekin daun teh hitam dan ekstrak aseton teh hitam dari tanaman *Camellia sinensis* var. *assamica*. *Jurnal Kimia, 14*(1), 43–52. https://doi.org/10.24843/jchem.2020.v14.i01.p08

Peitzika, S.-C., & Pontiki, E. (2023). A review on recent approaches on molecular docking studies of novel compounds targeting acetylcholinesterase in Alzheimer disease. *Molecules, 28*(3), 1084. https://doi.org/10.3390/molecules28031084

Pervin, M., Unno, K., Takagaki, A., Isemura, M., & Nakamura, Y. (2018). *Function of green tea catechins in the brain: Epigallocatechin gallate and its metabolites*. International Journal of Molecular Sciences, 19(11), 3630. https://doi.org/10.3390/ijms19113630

Pinzi, L., & Rastelli, G. (2019). *Molecular Docking: Shifting Paradigms in Drug Discovery.* International Journal of Molecular Sciences, 20(18), 4331. https://pmc.ncbi.nlm.nih.gov/articles/PMC6769923/

Pratama, F., Ruswanto, R., Nofianti, T., Tri, A., Pratita, K., & Daruwati, I. (2024). Radiolabeling and In-Silico Study of 131 I- ( 4-fluorobenzoyl-3-methylthiourea ) as Radiopharmaceuticals for Breast Cancer Theranostics. https://Journal.Uinjkt.Ac.Id/Orang.Php/Valensi, 18. https://doi.org/10.15408/jkv.v10i1.34258

Ravi, L., & Krishnan, K. (2016). A Handbook on Protein-Ligand Docking Tool: Autodock4. *Innovare Journal of Medical Science*, *4*(3), 1–6.

Renadi, S., Pratita, A. T. K., Mardianingrum, R., & Ruswanto, dan R. (2023). The Orang 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

Ruswanto, R., Mardianingrum, R., & Yanuar, A. (2022). Computational Studies of Thiourea Derivatives as Anticancer Candidates through Inhibition of Sirtuin1 (SIRT1). Jurnal Kimia Sains Dan Aplikasi, 25(3), 87–96. https://doi.org/10.14710/jksa.25.3.87-96

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(Orang), 15–36. https://doi.org/10.2147/AABC.S392068

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

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. Orang Journal of Scientific and Research Publications (IJSRP), 9(6), p90119. https://doi.org/10.29322/ijsrp.9.06.2019.p90119

Shi, M., et al. (2022). Molecular Docking, Molecular Dynamics Simulations, and Free Energy Calculation Insights into the Binding Mechanism between VS-4718 and Focal Adhesion Kinase. *ACS Omega*, 7(36), 32442–32456.

Sobolev, O. V., Afonine, P. V., Moriarty, N. W., Hekkelman, M. L., Joosten, R. P., Perrakis, A., & Adams, P. D. (2020). A global Ramachandran score identifies protein structures with unlikely stereochemistry. *Structure, 28*(11), 1249–1258.e2. https://doi.org/10.1016/j.str.2020.08.005

STRiDE Indonesia. (2023). *Prevalence and impacts of dementia in Indonesia.* STRiDE Project Report.

Sulimov, A., Kutov, D., Ilin, I., Sulimov, V., & Oferkin, I. (2022). *Quantum-chemical quasi-docking for molecular dynamics calculations*. *Nanomaterials, 12*(2), 274. https://doi.org/10.3390/nano12020274

Suriastini, N. W., Turana, Y., Witoelar, F., Supraptilah, B., Wicaksono, T. Y., & Endra, D. M. (2016). *Angka prevalensi demensia: Perlu perhatian kita semua.* Yogyakarta: SurveyMETER & Alzheimer's Indonesia Scientific Committee. https://media.neliti.com/media/publications/283-ID-angka-prevalensi-demensia-perlu-perhatian-kita-semua.pd

Syamsudin, R. A. M. R., Rustamsyah, A., Fadhlillah, F. M., Perdana, F., Inayah, A. A., & Abdul Aziz, M. Z. (2021). The effect of processing methods on characteristic, phenolic content, flavonoid content, and antioxidant activity of Garut traditional tea (kejek tea). *Jurnal Ilmiah Farmako Bahari, 12*(1), 69–79.

Tinworth, C. P., & Young, R. J. (2020). Drug-like properties and the design of orally bioavailable medicines. *Medicinal Chemistry Communications, 11*(8), 1234–1245.

Utami, D. P., Nurhayati, T., & Rahmawati, F. (2024). *In silico screening of bioactive compounds from Moringa oleifera against acetylcholinesterase using molecular docking, ADMET, and molecular dynamics approaches*. Journal of Biomolecular Structure and Dynamics, 42(12).

Velankar, S., Burley, S. K., Kurisu, G., Hoch, J. C., & Markley, J. L. (2021). Structural Proteomics High-Troughtput Methods. In R. J. Owens (Ed.), Nature Reviews Drug Discovery. Humana press. https://doi.org/https://doi.org/10.1007/978-1-0716-1406-8

Vieira, T. F., & Sousa, S. F. (2019). Comparing AutoDock and Vina in ligand/decoy discrimination for virtual screening. *Applied Sciences (Switzerland)*, *9*(21). https://doi.org/10.3390/app9214538

Wibowo, N. K., Rudyanto, M., & Purwanto, D. A. (2022). Aktivitas antioksidan teh hijau dan teh hitam. *Camellia: Clinical, Pharmaceutical, Analytical and Pharmacy Community Journal, 1*(2), 48–55.

Wijanarko, B. A., Puspitasari, L., & Bahri, S. (2026). Studi molecular docking senyawa flavonoid quercetin daun mimba (*Azadirachta indica* A. Juss) sebagai antidiabetes dan antioksidan. *Generics : Journal of Research in Pharmacy*, 6(1), 1-10. e-ISSN: 2774-9967.

World Health Organization. (2021). *Global status report on the public health response to dementia 2021*. World Health Organization. https://www.who.int/publications/i/item/9789240033245

Worldwide Protein Data Bank. (2023). *Validation report for PDB ID 4EY7*. RCSB Protein Data Bank. https://www.rcsb.org/structure/4EY7

Yassmine, H., Belaidi, S., Bourougaa, L., Ouassaf, M., Sinha, L., Samadi, A., & Chtita, S. (2023). *Identification of potent acetylcholinesterase inhibitors as new candidates for Alzheimer's disease via virtual screening, molecular docking, dynamic simulation, and MM-PBSA calculations. Molecules, 29*(6), 1232. https://doi.org/10.3390/molecules29061232

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

Yu, X., Zhang, Y., Zhang, M., Chen, Y., & Yang, W. (2022). *Natural products as sources of acetylcholinesterase inhibitors: Synthesis, biological activities, and molecular docking studies of osthole-based ester derivatives. Frontiers in Plant Science, 13,* 1054650. https://doi.org/10.3389/fpls.2022.1054650

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

Zhang, J., et al. (2024). Recent advances in Alzheimer's disease: mechanisms, diagnostics, and therapeutics. Signal Transduction and Targeted Therapy.

Zhang, J., Zhang, Y., Wang, J., Xia, Y., Zhang, J., & Chen, L. (2024). Recent advances in Alzheimer's disease: mechanisms, clinical trials and new drug development strategies. *Signal Transduction and Targeted Therapy, 9*(211). https://doi.org/10.1038/s41392-024-01911-3

Zhao, T., & Song, X. (2022). *Green Tea (Camellia sinensis): A Review of Its Phytochemistry, Pharmacology, and Toxicology.* Molecules, 27(12), 3909.