DAFTAR PUSTAKA

Ahmed, S., Khan, S. T., Zargaham, M. K., Khan, A. U., Khan, S., Hussain, A., … Al-Harrasi, A. (2021). Potential Therapeutic Natural Products Against Alzheimer's Disease with Reference of Acetylcholinesterase. *Biomedicine and Pharmacotherapy*, *139*, 1–23. https://doi.org/10.1016/j.biopha.2021.111609

Alqahtani, M. S., Kazi, M., Alsenaidy, M. A., & Ahmad, M. Z. (2021). Advances in Oral Drug Delivery. *Frontiers in Pharmacology*, *12*, 1–21. https://doi.org/10.3389/fphar.2021.618411

Arulanandam, C. D., Hwang, J.-S., Rathinam, A. J., & Dahms, H. U. (2022). Evaluating Different Web Applications to Assess the Toxicity of Plasticizers. *Scientific Reports*, *12*(1), 1–8. https://doi.org/10.1038/s41598-022-18327-0

Arya, A., Chahal, R., Rao, R., Rahman, M. H., Kaushik, D., Akhtar, M. F., … Mittal, V. (2021). Acetylcholinesterase Inhibitory Potential of Various Sesquiterpene Analogues for Alzheimer's Disease Therapy. *Biomolecules*, *11*(3), 1–30. https://doi.org/10.3390/biom11030350

Banerjee, P., Eckert, A. O., Schrey, A. K., & Preissner, R. (2018). ProTox-II: A Webserver for the Prediction of Toxicity of Chemicals. *Nucleic Acids Research*, *46*, 257–263. https://doi.org/10.1093/nar/gky318

Basnet, R., Khadka, S., Basnet, B. B., & Gupta, R. (2020). Perspective on Acetylcholinesterase: A Potential Target for Alzheimer's Disease Intervention. *Current Enzyme Inhibition*, *16*(3), 1–8. https://doi.org/10.2174/1573408016999200801021329

Berchansky, A., & Sussman, J. L. (2018). Human Acetylcholinesterase. Retrieved June 22, 2023, from Proteopedia website: https://proteopedia.org/wiki/index.php/Human_Acetylcholinesterase

Birks, J. S., & Harvey, R. J. (2018). Donepezil for Dementia due to Alzheimer's Disease. *Cochrane Database of Systematic Reviews*, (6), 1–245. https://doi.org/10.1002/14651858.CD001190.pub3

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

Burley, S. K., Berman, H. M., Duarte, J. M., Feng, Z., Flatt, J. W., Hudson, B. P., … Zardecki, C. (2022). Protein Data Bank: A Comprehensive Review of 3D Structure Holdings and Worldwide Utilization by Researchers, Educators, and Students. *Biomolecules*, *12*(10), 1–27. https://doi.org/10.3390/biom12101425

Carbone, J., Ghidini, A., Romano, A., Gentilucci, L., & Musiani, F. (2022). PacDOCK: A Web Server for Positional Distance-Based and Interaction-

Based Analysis of Docking Results. *Molecules*, *27*(20), 1–12. https://doi.org/10.3390/molecules27206884

Chakraborti, S., Hatti, K., & Srinivasan, N. (2021). 'All That Glitters Is Not Gold': High-Resolution Crystal Structures of Ligand-Protein Complexes Need Not Always Represent Confident Binding Poses. *International Journal of Molecular Sciences*, *22*(13), 1–26. https://doi.org/10.3390/ijms22136830

Chang, A., Vannabouathong, C., & Perras, C. (2022). Utilization of Cholinesterase Inhibitors for Alzheimer Disease in Canada. *Canadian Journal of Health Technologies*, *2*(6), 1–29. https://doi.org/10.51731/cjht.2022.361

Chikhale, H. U. (2020). Review on in-Silico Techniques: An Approach to Drug Discovery. *Current Trends in Pharmacy and Pharmaceutical Chemistry*, *2*(1), 24–32.

Daina, A., Michielin, O., & Zoete, V. (2017). SwissADME: A Free Web Tool to Evaluate Pharmacokinetics, Drug-Likeness and Medicinal Chemistry Friendliness of Small Molecules. *Scientific Reports*, *7*, 1–13. https://doi.org/10.1038/srep42717

Daina, A., & Zoete, V. (2019). Application of the SwissDrugDesign Online Resources in Virtual Screening. *International Journal of Molecular Sciences*, *20*(18), 1–12. https://doi.org/10.3390/ijms20184612

Dassault Systemes BIOVIA. (2021). *Biovia Discovery Studio ® 2018 Comprehensive Modeling and Simulations*. The 3DExperience® Company. Retrieved from accelrys.com/products/collaborative-science/biovia-discoverystudio

Dhorajiwala, T. M., Halder, S. T., & Samant, L. (2019). Comparative in Silico Molecular Docking Analysis of L-Threonine-3-Dehydrogenase, a Protein Target Against African Trypanosomiasis Using Selected Phytochemicals. *Journal of Applied Biotechnology Reports*, *6*(3), 101–108. https://doi.org/10.29252/JABR.06.03.04

Dnyandev, K. M., Babasaheb, G. V., Chandrashekhar, K. V., Chandrakant, M. A., & Vasant, O. K. (2021). A Review on Molecular Docking. *International Research Journal of Pure and Applied Chemistry*, *22*(3), 60–68. https://doi.org/10.9734/irjpac/2021/v22i330396

Dubach, V. R. A., & Guskov, A. (2020). The Resolution in X-ray Crystallography and Single-Particle Cryogenic Electron Microscopy. *Crystals*, *10*(7), 1–13. https://doi.org/10.3390/cryst10070580

Eberhardt, J., Santos-martins, D., Tillack, A. F., & Forli, S. (2021). AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. *Journal of Chemical Information and Modeling*, 1–7.

Erhirhie, E. O., Ihekwereme, C. P., & Ilodigwe, E. E. (2018). Advances in Acute

Toxicity Testing: Strengths, Weaknesses and Regulatory Acceptance. *Interdisciplinary Toxicology*, *11*(1), 5–12. https://doi.org/10.2478/intox-2018-0001

Falcón-Cano, G., Molina, C., & Cabrera-Pérez, M. Á. (2022). Reliable Prediction of Caco-2 Permeability by Supervised Recursive Machine Learning Approaches. *Pharmaceutics*, *14*(10), 1–21. https://doi.org/10.3390/pharmaceutics14101998

Gautam, B. (2020). Energy Minimization. In *Homology Molecular Modeling - Perspectives and Applications* (pp. 1–15). Prayagraj: IntechOpen. https://doi.org/10.5772/intechopen.94809

Gauthier, S., Webster, C., Servaes, S., Morais, J. A., & Rosa-Neto, P. (2022). *World Alzheimer Report 2022 - Life after Diagnosis: Navigating Treatment, Care and Support* (C. Benoist & W. Weidner, Eds.). London, England: Alzheimer's Disease International. Retrieved from https://www.alz.co.uk/research/WorldAlzheimerReport2015.pdf

Ghani, S. S. (2020). A Comprehensive Review of Database Resources in Chemistry. *Eclética Química*, *45*(3), 57–68. https://doi.org/https://doi.org/10.26850/1678-4618eqj.v45.3.2020.p57-68

Gilman, E. F., Watson, D. G., Klein, R. W., Koeser, A. K., Hilbert, D. R., & Mclean, D. C. (2018). Ginkgo biloba: Ginkgo. *UF/IFAS Extension*, 1–3.

Gu, Y. (2022). Effect of Ginkgo Biloba Extract (EGb761) on Cerebral Nervous System in Patients with ALzheimer's Disease. *International Seminar on Education, Management and Social Sciences (ISEMSS)*, 267–273. https://doi.org/10.2991/978-2-494069-31-2

Hampel, H., Mesulam, M. M., Cuello, A. C., Farlow, M. R., Giacobini, E., Grossberg, G. T., … Khachaturian, Z. S. (2018). The Cholinergic System in the Pathophysiology and Treatment of Alzheimer's Disease. *Brain*, *141*(7), 1917–1933. https://doi.org/10.1093/brain/awy132

HV, S., Raj, A., K, G., S, C., & K, S. (2020). Kinetics and Computational Analysis of Cholinesterase Inhibition by REVERC3, a Bisdemethoxycurcumin-rich Curcuma longa Extract: Relevance to the Treatment of Alzheimer's Disease. *SAGE Open Medicine*, *8*, 1–9. https://doi.org/10.1177/2050312120973499

Ivanović, V., Rančić, M., Arsić, B., & Pavlović, A. (2020). Lipinski's Rule of Five, Famous Extensions and Famous Exceptions. *Popular Scientific Article*, *3*(1), 171–177.

Juvale, I. I. A., Hamid, A. A. A., Halim, K. B. A., & Has, A. T. C. (2022). P-Glycoprotein: New Insights into Structure, Physiological Function, Regulation and Alterations in Disease. *Heliyon*, *8*(6), 1–12. https://doi.org/10.1016/j.heliyon.2022.e09777

Kabra, A., & Ramteke, A. (2021). Alzheimer Disease – Etiology, Pathophysiology and Treatment: An Overview. *Annals of the Romanian Society for Cell Biology*, *25*(1), 3548–3556. Retrieved from https://www.annalsofrscb.ro/index.php/journal/article/view/465

Kumar, A., Sharma, A., Kaur, H., Punera, S., Tanwar, P., & Kumar, P. (2021). Interaction of Protein-Ligand: Molecular Docking, A Novel Computational Biology Tool. *Annals of the Romanian Society for Cell Biology*, *25*(6), 20763–20775. Retrieved from https://www.researchgate.net/publication/356033779

Kunzmann, P., Anter, J. M., & Hamacher, K. (2022). Adding Hydrogen Atoms to Molecular Models via Fragment Superimposition. *Algorithms for Molecular Biology*, *17*(1), 1–8. https://doi.org/10.1186/s13015-022-00215-x

Kurisu, G. (2022). Fifty years of Protein Data Bank in the Journal of Biochemistry. *Journal of Biochemistry*, *171*(1), 3–11. https://doi.org/10.1093/jb/mvab133

Kurniawidjaja, L. M., Lestari, F., Tejamaya, M., & Ramdhan, D. H. (2021). Konsep Dasar Toksikologi Industri. In *Fkm Ui* (1st ed.). Depok: Fakultas Kesehatan Masyarakat Universitas Indonesia.

Lange, E. C. M. de, & Udenaes, M. H. (2022). Understanding the Blood-Brain Barrier and Beyond: Challenges and Opportunities for Novel CNS Therapeutics. *Clinical Pharmacology and Therapeutics*, *111*(4), 758–773. https://doi.org/10.1002/cpt.2545

Liu, H., Ye, M., & Guo, H. (2020). An Updated Review of Randomized Clinical Trials Testing the Improvement of Cognitive Function of Ginkgo biloba Extract in Healthy People and Alzheimer's Patients. *Frontiers in Pharmacology*, *10*, 1–8. https://doi.org/10.3389/fphar.2019.01688

Makarian, M., Gonzalez, M., Salvador, S. M., Lorzadeh, S., Hudson, P. K., & Pecic, S. (2022). Synthesis, Kinetic Evaluation and Molecular Docking Studies of Donepezil-Based Acetylcholinesterase Inhibitors. *Journal of Molecular Structure*, *1247*, 1–24. https://doi.org/10.1016/j.molstruc.2021.131425

Makrynitsa, G. I., Lykouras, M., Spyroulias, G. A., & Matsoukas, M. (2018). In Silico Drug Design. *ELS*, 1–7. https://doi.org/10.1002/9780470015902.a0028112

Marques, J. M. C., Prudente, F. V., & Pirani, F. (2022). Intermolecular Forces: From Atoms and Molecules to Nanostructures. *Molecules*, *27*(10), 1–3. https://doi.org/10.3390/molecules27103072

Marucci, G., Buccioni, M., Ben, D. D., Lambertucci, C., Volpini, R., & Amenta, F. (2021). Efficacy of Acetylcholinesterase Inhibitors in Alzheimer's Disease. *Neuropharmacology*, *190*, 1–15.

https://doi.org/10.1016/j.neuropharm.2020.108352

Matsson, P., & Kihlberg, J. (2017). How Big Is Too Big for Cell Permeability? *Journal of Medicinal Chemistry*, *60*(5), 1662–1664. https://doi.org/10.1021/acs.jmedchem.7b00237

Mohsin, N. U. A., & Ahmad, M. (2020). Donepezil: A Review of the Recent Structural Modifications and Their Impact on Anti-Alzheimer Activity. *Brazilian Journal of Pharmaceutical Sciences*, *56*, 1–16. https://doi.org/10.1590/S2175-97902019000418325

Muchtaridi, Yusuf, M., & Megantara, S. (2017). *Penambatan Molekul (Molecular Docking)* (1st ed.). Yogyakarta: Deepublish.

Murugan, N. A., Podobas, A., Gadioli, D., Vitali, E., Palermo, G., & Markidis, S. (2022). A Review on Parallel Virtual Screening Softwares for High-Performance Computers. *Pharmaceuticals*, *15*(1), 1–33. https://doi.org/10.3390/ph15010063

NCERT. (2020). *Chemistry - Part 1*. India: NCERT.

Nguyen, D., Xiao, T., Wang, M., & Wei, G. (2018). Rigidity Strengthening Is a Vital Mechanism for Protein-Ligand Binding. *Biomolecules*, 1–10. https://doi.org/10.48550/arXiv.1704.05883

Nowak, A., Kojder, K., Zielonka-Brzezicka, J., Wróbel, J., Bosiacki, M., Fabiańska, M., … Klimowicz, A. (2021). The Use of Ginkgo Biloba L. as a Neuroprotective Agent in the Alzheimer's Disease. *Frontiers in Pharmacology*, *12*, 1–18. https://doi.org/10.3389/fphar.2021.775034

Pantaleão, S. Q., Fernandes, P. O., Gonçalves, J. E., Maltarollo, V. G., & Honorio, K. M. (2022). Recent Advances in the Prediction of Pharmacokinetics Properties in Drug Design Studies: A Review. *ChemMedChem*, *17*(1), 1–13. https://doi.org/https://doi.org/10.1002/cmdc.202100542

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), 1–28. https://doi.org/10.3390/molecules28031084

Prieto-Martínez, F. D., Arciniega, M., & Medina-Franco, J. L. (2018). Molecular Docking: Current Advances and Challenges. *TIP Revista Especializada En Ciencias Químico-Biológicas*, *21*(1), 65–87. https://doi.org/10.22201/fesz.23958723e.2018.0.143

Rantih, N. K., Mulyani, S., & Widhiyanti, T. (2019). An Analyses of Multiple Representation about Intermolecular Forces. *Journal of Physics: Conference Series*, 1–7. https://doi.org/10.1088/1742-6596/1157/4/042029

Rout, S. K., Nikhat, F., & Mohanty, S. (2022). In Silico Molecular Docking Analysis of Potential Anti-Alzheimer's Compounds Present in Occimum Santum. *International Journal of Drug Development and Research*, *14*(9:

977), 1–6. https://doi.org/10.36648-0975-9344-14.09-977

Sampat, G., Suryawanshi, S. S., Palled, M. S., Patil, A. S., Khanal, P., & Salokhe, A. S. (2022). Drug Likeness Screening and Evaluation of Physicochemical Properties of Selected Medicinal Agents by Computer Aided Drug Design Tools. *Advances in Pharmacology and Pharmacy*, *10*(4), 234–246. https://doi.org/10.13189/app.2022.100402

Sen, D. J., Nandi, K., & Saha, D. (2021). Rule of Five: the Five Men Army to Cross the Blood Brain Barrier for Therapeutically Potent. *World Journal of Advance Healthcare Research*, *5*(3), 206–211. Retrieved from https://www.researchgate.net/publication/351945081

Sharma, K. (2019). Cholinesterase Inhibitors as Alzheimer's Therapeutics (Review). *Molecular Medicine Reports*, *20*(2), 1479–1487. https://doi.org/10.3892/mmr.2019.10374

Sinyor, B., Mineo, J., & Ochner, C. (2020). Alzheimer's Disease, Inflammation, and the Role of Antioxidants. *Journal of Alzheimer's Disease Reports*, *4*(1), 175–183. https://doi.org/10.3233/adr-200171

Stanciu, G. D., Luca, A., Rusu, R. N., Bild, V., Chiriac, S. I. B., Solcan, C., … Ababei, D. C. (2020). Alzheimer's Disease Pharmacotherapy in Relation to Cholinergic System Involvement. *Biomolecules*, *10*(1), 1–21. https://doi.org/10.3390/biom10010040

Strickland, J., Paris, M. W., Allen, D., & Casey, W. (2019). Approaches to Reducing Animal Use for Acute Toxicity Testing: Retrospective Analyses of Pesticide Data. In H. Kojima, T. Seidle, & H. Spielmann (Eds.), *Alternatives to Animal Testing* (pp. 37–49). Singapura: Springer Open. https://doi.org/10.1007/978-981-13-2447-5_11

Trott, O., & Olson, A. J. (2010). 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.

Tsatsakis, A. M., Vassilopoulou, L., Kovatsi, L., Tsitsimpikou, C., Karamanou, M., Leon, G., … Spandidos, D. A. (2018). The Dose Response Principle from Philosophy to Modern Toxicology: The Impact of Ancient Philosophy and Medicine in Modern Toxicology Science. *Toxicology Reports*, *5*, 1107–1113. https://doi.org/10.1016/j.toxrep.2018.10.001

Uddin, M. S., Kabir, M. T., Niaz, K., Jeandet, P., Clément, C., Mathew, B., … Aleya, L. (2020). Molecular Insight into the Therapeutic Promise of Flavonoids Against Alzheimer's Disease. *Molecules*, *25*(6), 1–29. https://doi.org/10.3390/molecules25061267

Xie, L., Zhu, Q., & Lu, J. (2022). Can We Use Ginkgo biloba Extract to Treat Alzheimer's Disease? Lessons from Preclinical and Clinical Studies. *Cells*, *11*(3), 1–26. https://doi.org/10.3390/cells11030479

Yuliyanto, E., & Hidayah, F. F. (2018). *Buku Ajar_Kimia Organik: Asam Karboksilat Berbasis Software Marvin Plus Refleksi*. Semarang: Unimus Press. Retrieved from http://repository.unimus.ac.id/3936/1/Buku Ajar PrakTikum Kimia Organik Berbasis Marvin.pdf

Yunta, M. J. R. (2017). It Is Important to Compute Intramolecular Hydrogen Bonding in Drug Design? *American Journal of Modeling and Optimization*, *5*(1), 24–57. https://doi.org/10.12691/ajmo-5-1-3

Zeng, P., Fang, M., Zhao, H., & Guo, J. (2021). A Network Pharmacology Approach to Uncover the Key Ingredients in Ginkgo folium and Their Anti-Alzheimer's Disease Mechanisms. *Aging*, *13*(14), 18993–19012. https://doi.org/10.18632/aging.203348

Zothantluanga, J. H., & Chetia, D. (2022). A Beginner's Guide to Molecular Docking. *Sciences of Phytochemistry*, *1*(2), 37–40. https://doi.org/10.58920/sciphy01020037