

## DAFTAR PUSTAKA

- Aris, P., Mohamadzadeh, M., Wei, Y., & Xia, X. (2022). In Silico Molecular Dynamics of Griseofulvin and Its Derivatives Revealed Potential Therapeutic Applications for COVID-19. *International Journal of Molecular Sciences*, 23(13), 6889. <https://doi.org/10.3390/ijms23136889>
- Arnittali, M., Rissanou, A. N., & Harmandaris, V. (2019). Structure Of Biomolecules Through Molecular Dynamics Simulations. *Procedia Computer Science*, 156, 69–78. <https://doi.org/10.1016/j.procs.2019.08.181>
- Aswad, M., Christine, L., Nursamsiar, N., & Hardianti, B. (2020). Studi Penambatan Molekul Senyawa-Senyawa Bioaktif Dari Kulit Akar Murbei (*Morus Sp.*) Terhadap Reseptor Tnf-A. *Majalah Farmasi dan Farmakologi*, 23(3), 85–100. <https://doi.org/10.20956/mff.v23i3.9399>
- Az-Zahra, F., Afidika, J., Diamantha, S. D. A., Rahmani, A. E., 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).
- Bell, E. W., & Zhang, Y. (2019). DockRMSD: An open-source tool for atom mapping and RMSD calculation of symmetric molecules through graph isomorphism. *Journal of Cheminformatics*, 11(1), 40. <https://doi.org/10.1186/s13321-019-0362-7>
- Breberina, L. M., Zlatović, M. V., Nikolić, M. R., & Stojanović, S. Đ. (2019). Computational Analysis of Non-covalent Interactions in Phycocyanin Subunit Interfaces. *Molecular Informatics*, 38(11–12), 1800145. <https://doi.org/10.1002/minf.201800145>
- 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, 612. <https://doi.org/10.3389/fchem.2020.00612>
- 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), 6884. <https://doi.org/10.3390/molecules27206884>
- Cardoso, W. B., & Mendanha, S. A. (2021). Molecular dynamics simulation of docking structures of SARS-CoV-2 main protease and HIV protease inhibitors. *Journal of Molecular Structure*, 1225, 129143. <https://doi.org/10.1016/j.molstruc.2020.129143>
- Chen, J., Song, J., Yuan, P., Tian, Q., Ji, Y., Ren-Patterson, R., Liu, G., Sei, Y., & Weinberger, D. R. (2011). Orientation and Cellular Distribution of Membrane-bound Catechol-O-methyltransferase in Cortical Neurons.

- Journal of Biological Chemistry*, 286(40), 34752–34760. <https://doi.org/10.1074/jbc.M111.262790>
- Chikhale, H. U. (2020). Review on In-silico techniques: An approach to Drug discovery. *Department of Pharmaceutical Chemistry, Gokhale Education Society's Sir*, 2(1).
- Coumar, M. S. (Ed.). (2021). *Molecular docking for computer-aided drug design: Fundamentals, techniques, resources and applications*. Academic Press.
- Dhorajiwala, T., Halder, S., & 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>
- DiPiro, J. T., Yee, G. C., Posey, L. M., Haines, S. T., Nolin, T. D., & Ellingrod, V. (2020). *Pharmacotherapy: A pathophysiologic approach* (11 th). McGraw Hill.
- Diyan, D. S. P., Hari Susanti, & Nining Sugihartini. (2021). Molecular Docking As Potential Anti-Inflamed Quersetin Of Moringa Leaves (*Moringa Oleifera* L.) With Autodock-Vina. *Jurnal Ilmiah Manusia Dan Kesehatan*, 4(2), 309–313. <https://doi.org/10.31850/makes.v4i2.818>
- 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*, 60–68. <https://doi.org/10.9734/irjpac/2021/v22i330396>
- Do, H. T. T., & Cho, J. (2020). Mangosteen Pericarp and Its Bioactive Xanthenes: Potential Therapeutic Value in Alzheimer's Disease, Parkinson's Disease, and Depression with Pharmacokinetic and Safety Profiles. *International Journal of Molecular Sciences*, 21(17), 6211. <https://doi.org/10.3390/ijms21176211>
- dos Santos Passos, C., Klein-Júnior, L. C., de Mello Andrade, J. M., Matté, C., & Henriques, A. T. (2015). The catechol-O-methyltransferase inhibitory potential of Z-vallesiachotamine by in silico and in vitro approaches. *Revista Brasileira de Farmacognosia*, 25(4), 382–386. <https://doi.org/10.1016/j.bjp.2015.07.002>
- 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>
- Esmail, S. (2018). The Diagnosis and Management of Parkinson's Disease. *Scholar Journal of Applied Sciences and Research*, 1.
- Fatriansyah, J. F., Boanerges, A. G., Kurnianto, S. R., Pradana, A. F., Fadilah, & Surip, S. N. (2022). Molecular Dynamics Simulation of Ligands from *Anredera cordifolia* (Binahong) to the Main Protease (Mpro) of SARS-CoV-

2. *Journal of Tropical Medicine*, 2022, 1–13.  
<https://doi.org/10.1155/2022/1178228>
- Febrina, D., & Milanda, T. (2018). PHARMACOLOGICAL ACTIVITY *Garcinia mangostana* LINN : A REVIEW. *International Journal of Current Medical Sciences*, 8.
- Genheden, S., & Ryde, U. (2015). The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. *Expert Opinion on Drug Discovery*, 10(5), 449–461. <https://doi.org/10.1517/17460441.2015.1032936>
- Ghahremanian, S., Rashidi, M. M., Raeisi, K., & Toghraie, D. (2022). Molecular dynamics simulation approach for discovering potential inhibitors against SARS-CoV-2: A structural review. *Journal of Molecular Liquids*, 354, 118901. <https://doi.org/10.1016/j.molliq.2022.118901>
- Gnanaraj, C., Sekar, M., Fuloria, S., Swain, S. S., Gan, S. H., Chidambaram, K., Rani, N. N. I. M., Balan, T., Stephenie, S., Lum, P. T., Jeyabalan, S., Begum, M. Y., Chandramohan, V., Thangavelu, L., Subramaniyan, V., & Fuloria, N. K. (2022). In Silico Molecular Docking Analysis of Karanjin against Alzheimer's and Parkinson's Diseases as a Potential Natural Lead Molecule for New Drug Design, Development and Therapy. *Molecules*, 27(9), 2834. <https://doi.org/10.3390/molecules27092834>
- Govindasamy, H., Magudeeswaran, S., & Poomani, K. (2020). Identification of novel flavonoid inhibitor of Catechol-O-Methyltransferase enzyme by molecular screening, quantum mechanics/molecular mechanics and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, 38(18), 5307–5319. <https://doi.org/10.1080/07391102.2019.1699446>
- Habet, S. (2022). Clinical Pharmacology of Entacapone (Comtan) From the FDA Reviewer. *International Journal of Neuropsychopharmacology*, 25(7), 567–575. <https://doi.org/10.1093/ijnp/pyac021>
- Haider, A., Elghazawy, N. H., Dawoud, A., Gebhard, C., Wichmann, T., Sippl, W., Hoener, M., Arenas, E., & Liang, S. H. (2023). Translational molecular imaging and drug development in Parkinson's disease. *Molecular Neurodegeneration*, 18(1), 11. <https://doi.org/10.1186/s13024-023-00600-z>
- Hayes, M. T. (2019). Parkinson's Disease and Parkinsonism. *The American Journal of Medicine*, 132(7), 802–807. <https://doi.org/10.1016/j.amjmed.2019.03.001>
- 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>
- Iijima, H., Takebe, K., Suzuki, M., Kobayashi, H., Takamiya, T., Saito, H., Niwa, N., & Kuwada-Kusunose, T. (2020). Crystal Structure of Catechol O-Methyltransferase Complexed with Nitecapone. *Chemical and*

- Pharmaceutical Bulletin*, 68(5), 447–451. <https://doi.org/10.1248/cpb.c20-00011>
- Ishak, N. I., La Kilo, A., Halidi, D. S., Aman, L. O., La Kilo, J., & Musa, W. J. A. (2023). Molecular Docking of Secondary Metabolite Compounds of *Andrographis Paniculata* Plant as Potential Covid-19 Drug Candidate. *Jurnal Sains Dan Kesehatan*, 5(3). <https://doi.org/10.25026/jsk.v5i3.1845>
- Jankovic, J., & Tan, E. K. (2020). Parkinson's disease: Etiopathogenesis and treatment. *Journal of Neurology, Neurosurgery & Psychiatry*, 91(8), 795–808. <https://doi.org/10.1136/jnnp-2019-322338>
- Jawd, S. M., Sabea, A. M., & Chekhyor, N. H. (2021). *Review on Parkinson's Disease (Causes, Symptoms, Diagnosis, Treatment)*.
- Jenner, P., Rocha, J.-F., Ferreira, J. J., Rascol, O., & Soares-da-Silva, P. (2021). Redefining the strategy for the use of COMT inhibitors in Parkinson's disease: The role of opicapone. *Expert Review of Neurotherapeutics*, 21(9), 1019–1033. <https://doi.org/10.1080/14737175.2021.1968298>
- Khaw, K. Y., Chong, C. W., & Murugaiyah, V. (2020). LC-QTOF-MS analysis of xanthone content in different parts of *Garcinia mangostana* and its influence on cholinesterase inhibition. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 35(1), 1433–1441. <https://doi.org/10.1080/14756366.2020.1786819>
- Klemann, C. J. H. M., Martens, G. J. M., Sharma, M., Martens, M. B., Isacson, O., Gasser, T., Visser, J. E., & Poelmans, G. (2017). Integrated molecular landscape of Parkinson's disease. *Npj Parkinson's Disease*, 3(1), 14. <https://doi.org/10.1038/s41531-017-0015-3>
- Kolina, J., Sumiwi, S. A., & Levita, J. (2019). MODE IKATAN METABOLIT SEKUNDER DI TANAMAN AKAR KUNING (*Arcangelisia flava* L.) DENGAN NITRAT OKSIDA SINTASE. *FITOFARMAKA: Jurnal Ilmiah Farmasi*, 8(1), 45–52. <https://doi.org/10.33751/jf.v8i1.1171>
- Lee, T. K., & Yankee, E. L. (2022). A review on Parkinson's disease treatment. *Neuroimmunology and Neuroinflammation*, 8, 222. <https://doi.org/10.20517/2347-8659.2020.58>
- Ma, Z., Liu, H., & Wu, B. (2014). Structure-based drug design of catechol-O-methyltransferase inhibitors for CNS disorders: Structure-based design of COMT inhibitors. *British Journal of Clinical Pharmacology*, 77(3), 410–420. <https://doi.org/10.1111/bcp.12169>
- Makatita, F. A., & Wardhani, R. (2020). Riset In Silico Dalam Pengembangan Sains Di Bidang Pendidikan, Studi Kasus: Analisis Potensi Cendana Sebagai Agen Anti-Aging. *Jurnal Abdi*, 2(1).
- Miller, B. R., McGee, T. D., Swails, J. M., Homeyer, N., Gohlke, H., & Roitberg, A. E. (2012). MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. *Journal of Chemical Theory and Computation*, 8(9), 3314–3321. <https://doi.org/10.1021/ct300418h>

- Misra, M., & Yadav, A. K. (2022). Assessment of Available AMBER Force Fields to Model DNA-Ligand Interactions. *Biointerface Research in Applied Chemistry*, 13(2), 156. <https://doi.org/10.33263/BRIAC132.156>
- Moradi, M., Golmohammadi, R., Najafi, A., Moosazadeh Moghaddam, M., Fasihi-Ramandi, M., & Mirnejad, R. (2022). A contemporary review on the important role of in silico approaches for managing different aspects of COVID-19 crisis. *Informatics in Medicine Unlocked*, 28, 100862. <https://doi.org/10.1016/j.imu.2022.100862>
- Nidyasari, Rr. S., Akmal, H., & Ariyanti, N. S. (2018). Karakterisasi Morfologi dan Anatomi Tanaman Manggis dan Kerabatnya (*Garcinia* spp.) di Taman Buah Mekarsari. *Jurnal Sumberdaya Hayati*, 4(1), 12–20. <https://doi.org/10.29244/jsdh.4.1.12-20>
- Nurrahma, B. A., Yeh, T.-H., Hsieh, R.-H., Tsao, S.-P., Chen, C.-W., Lee, Y.-P., Pan, C.-H., & Huang, H.-Y. (2022). Mangosteen Pericarp Extract Supplementation Boosts Antioxidant Status via Rebuilding Gut Microbiota to Attenuate Motor Deficit in 6-OHDA-Induced Parkinson's Disease. *Antioxidants*, 11(12), 2396. <https://doi.org/10.3390/antiox11122396>
- Oksanen, E., Chen, J. C.-H., & Fisher, S. Z. (2017). Neutron Crystallography for the Study of Hydrogen Bonds in Macromolecules. *Molecules*, 22(4), 596. <https://doi.org/10.3390/molecules22040596>
- Pantsar, T., & Poso, A. (2018). Binding Affinity via Docking: Fact and Fiction. *Molecules*, 23(8), 1899. <https://doi.org/10.3390/molecules23081899>
- Pitojo, S., & Puspita, H. N. (2007). *Budi Daya Manggis*. CV. Aneka Ilmu.
- Pratama, M. R. F., Poerwono, H., & Siswodihardjo, S. (2021). Introducing a two-dimensional graph of docking score difference vs. Similarity of ligand-receptor interactions. *Indonesian Journal of Biotechnology*, 26(1), 54. <https://doi.org/10.22146/ijbiotech.62194>
- R Desai, S., R Doke, R., A Pansare, P., R Sainani, S., & M Bhalchim, V. (2019). Natural products: An emerging tool in parkinson's disease therapeutics. *IP Indian Journal of Neurosciences*, 5(3), 95–105. <https://doi.org/10.18231/j.ijn.2019.014>
- Radhakrishnan, D., & Goyal, V. (2018). Parkinson's disease: A review. *Neurology India*, 66(7), 26. <https://doi.org/10.4103/0028-3886.226451>
- Rahman, Md. M., Wang, X., Islam, Md. R., Akash, S., Supti, F. A., Mitu, M. I., Harun-Or-Rashid, Md., Aktar, Most. N., Khatun Kali, Most. S., Jahan, F. I., Singla, R. K., Shen, B., Rauf, A., & Sharma, R. (2022). Multifunctional role of natural products for the treatment of Parkinson's disease: At a glance. *Frontiers in Pharmacology*, 13, 976385. <https://doi.org/10.3389/fphar.2022.976385>
- Rangaraju, A. (2013). Review On Molecular Docking– Novel tool in drug design and analysis. *Journal Of Harmonized Research (JOHR)*.

- Rath, S. N., Jena, L., Bhuyan, R., Mahanandia, N. C., & Patri, M. (2021). In silico discovery and evaluation of phytochemicals binding mechanism against human catechol-O-methyltransferase as a putative bioenhancer of L-DOPA therapy in Parkinson disease. *Genomics & Informatics*, *19*(1), e7. <https://doi.org/10.5808/gi.20061>
- Rizaldy, D., Hartati, R., Nadhifa, T., & Fidrianny, I. (2021). Chemical Compounds and Pharmacological Activities of Mangosteen (*Garcinia mangostana* L.) – Updated Review. *Biointerface Research in Applied Chemistry*, *12*(2), 2503–2516. <https://doi.org/10.33263/BRIAC122.25032516>
- Roger, B. F. (2020). Amantadine for the Treatment of Parkinson’s Disease and its Associated Dyskinesias. *Avens Publishing Group*, *7*(1).
- Saleem, S., Muhammad, G., Hussain, M. A., Altaf, M., & Bukhari, S. N. A. (2020). *Withania somnifera* L.: Insights into the phytochemical profile, therapeutic potential, clinical trials, and future prospective. *Iranian Journal of Basic Medical Sciences*, *23*(12). <https://doi.org/10.22038/ijbms.2020.44254.10378>
- Sari, I. W., Junaidin, J., & Pratiwi, D. (2020). Studi Molecular Docking Senyawa Flavonoid Herba Kumis Kucing (*Orthosiphon Stamineus* B.) Pada Reseptor A-Glukosidase Sebagai Antidiabetes Tipe 2. *Jurnal Farmagazine*, *7*(2), 54. <https://doi.org/10.47653/farm.v7i2.194>
- Scott, L. J. (2016). Opicapone: A Review in Parkinson’s Disease. *Drugs*, *76*(13), 1293–1300. <https://doi.org/10.1007/s40265-016-0623-y>
- Solayman, Md., Islam, Md., Alam, F., Khalil, Md., Kamal, M., & Gan, S. (2017). Natural Products Combating Neurodegeneration: Parkinson’s Disease. *Current Drug Metabolism*, *18*(1), 50–61. <https://doi.org/10.2174/1389200217666160709204826>
- Susanti, L., Mustarichie, R., Halimah, E., Kurnia, D., Setiawan, A., & Maladan, Y. (2022). Anti-Alopecia Activity of Alkaloids Group from Noni Fruit against Dihydrotestosterone-Induced Male Rabbits and Its Molecular Mechanism: In Vivo and In Silico Studies. *Pharmaceuticals*, *15*(12), 1557. <https://doi.org/10.3390/ph15121557>
- Swamy, M. K. (Ed.). (2020). *Plant-derived Bioactives: Chemistry and Mode of Action*. Springer Singapore. <https://doi.org/10.1007/978-981-15-2361-8>
- Syahputra, M. R., Setiado, H., Siregar, L. A. M., & Damanik, R. I. (2021). Morphological characteristics of Mangosteen plants (*Garcinia mangostana* L.) in Langkat District, North Sumatera, Indonesia. *IOP Conference Series: Earth and Environmental Science*, *782*(4), 042056. <https://doi.org/10.1088/1755-1315/782/4/042056>
- Syahputra, R., Utami, D., & Widyaningsih, W. (2022). Molecular Docking Study Of Tyrosinase Enzyme. *Jurnal Farmasi Indonesia*, *9*.

- Tan, Y.-Y., Jenner, P., & Chen, S.-D. (2022). Monoamine Oxidase-B Inhibitors for the Treatment of Parkinson's Disease: Past, Present, and Future. *Journal of Parkinson's Disease*, 12(2), 477–493. <https://doi.org/10.3233/JPD-212976>
- Wang, E., Sun, H., Wang, J., Wang, Z., Liu, H., Zhang, J. Z. H., & Hou, T. (2019). End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. *Chemical Reviews*, 119(16), 9478–9508. <https://doi.org/10.1021/acs.chemrev.9b00055>
- Wang, F.-Y., Wei, G.-L., Fan, Y.-F., Zhao, D.-F., Wang, P., Zou, L.-W., & Yang, L. (2021). Inhibition of catechol-O-methyltransferase by natural pentacyclic triterpenes: Structure–activity relationships and kinetic mechanism. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 36(1), 1079–1087. <https://doi.org/10.1080/14756366.2021.1928112>
- WHO. (2022). *Parkinson disease: A public health approach. Technical brief*. World Health Organization.
- Yamamoto, J., Omura, T., Kasamo, S., Yamamoto, S., Kawata, M., Yonezawa, A., Taruno, Y., Endo, H., Aizawa, H., Sawamoto, N., Matsubara, K., Takahashi, R., & Tasaki, Y. (2021). Impact of the catechol-O-methyltransferase Val158Met polymorphism on the pharmacokinetics of l-dopa and its metabolite 3-O-methyldopa in combination with entacapone. *Journal of Neural Transmission*, 128(1), 27–36. <https://doi.org/10.1007/s00702-020-02267-y>
- Yang, R., Li, P., Li, N., Zhang, Q., Bai, X., Wang, L., Xiao, Y., Sun, L., Yang, Q., & Yan, J. (2017). Xanthones from the Pericarp of *Garcinia mangostana*. *Molecules*, 22(5), 683. <https://doi.org/10.3390/molecules22050683>
- Yu, W., & MacKerell, A. D. (2017). Computer-Aided Drug Design Methods. In P. Sass (Ed.), *Antibiotics* (Vol. 1520, pp. 85–106). Springer New York. [https://doi.org/10.1007/978-1-4939-6634-9\\_5](https://doi.org/10.1007/978-1-4939-6634-9_5)
- Yusuf, M., Pratama, B. S. W., Baroroh, U., Ghaffar, S., & Soedjanaatmadj, U. M. (2022). Studi In Silico Gadolinium(III)-Diethylene Triamine Pentaacetic Acid-Folat Dan Modifikasinya Terhadap Reseptor Folat Sebagai Senyawa Pengontras Untuk Deteksi Kanker. *Chimica et Natura Acta*. <https://doi.org/10.24198/cna.v9.n3.36035>
- Zhao, D.-F., Fan, Y.-F., Wang, F.-Y., Hou, F.-B., Gonzalez, F. J., Li, S.-Y., Wang, P., Xia, Y.-L., Ge, G.-B., & Yang, L. (2021). Discovery and characterization of naturally occurring potent inhibitors of catechol- O -methyltransferase from herbal medicines. *RSC Advances*, 11(17), 10385–10392. <https://doi.org/10.1039/D0RA10425F>