

Daftar Pustaka

- Adiyasa, M.R. and Meiyanti, M. (2021) 'Pemanfaatan obat tradisional di Indonesia: distribusi dan faktor demografis yang berpengaruh', *Jurnal Biomedika dan Kesehatan*, 4(3), pp. 130–138. Available at: <https://doi.org/10.18051/JBiomedKes.2021.v4.130-138>.
- Alhusban, M., Pandey, P., Ahn, J., Avula, B., Haider, S., Avonto, C., Ali, Z., Khan, S.I., Ferreira, D., Khan, I.A. and Chittiboyina, A.G. (2022) 'Computational Tools to Expedite the Identification of Potential PXR Modulators in Complex Natural Product Mixtures: A Case Study with Five Closely Related Licorice Species', *ACS Omega*, 7(30), pp. 26824–26843. Available at: <https://doi.org/10.1021/acsomega.2c03240>.
- Alnaqeeb, M., Mansor, K.A., Mallah, E.M., Ghanim, B.Y., Idkaidek, N. and Qinna, N.A. (2019) 'Critical pharmacokinetic and pharmacodynamic drug-herb interactions in rats between warfarin and pomegranate peel or guava leaves extracts', *BMC Complementary and Alternative Medicine*, 19(1), p. 29. Available at: <https://doi.org/10.1186/s12906-019-2436-5>.
- Arianingrum, R., Hermawan, A., Purnomo, H., Dewi, D. and Meiyanto, E. (2019) 'Molecular Docking Studies of a Chalcone Derivative Compound *p* - hydroxy- *m* -methoxychalcone with Tyrosine Kinase Receptors', *Indian Journal of Public Health Research & Development*, 10(7), pp. 1219. Available at: <https://doi.org/10.5958/0976-5506.2019.01752.2>.
- Arwansyah & Hasrianti. (2015) 'Simulasi Molecular Docking Senyawa Kurkumin dan Analognya sebagai Selective Androgen Receptor Modulators (SARMs) pada Kanker Prostat', *Dinamika*, vol. 5, no. 2, pp. 60-75.
- Beny, R., Yana, N.R.A. and Leorita, M. (2020) 'Desain Turunan Senyawa Leonurine Sebagai Kandidat Obat Anti Inflamasi: Design of Leonurine Derivatives as Anti-Inflammatory Candidates', *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy) (e-Journal)*, 6(1), pp. 181–191. Available at: <https://doi.org/10.22487/j24428744.2020.v6.i1.15025>.
- Buchman, C.D., Chai, S.C. and Chen, T. (2018) 'A Current Structural Perspective on PXR and CAR in Drug Metabolism', *Expert Opinion on Drug Metabolism & Toxicology*, 14(6), pp. 635–647. Available at: <https://doi.org/10.1080/17425255.2018.1476488>.
- Chai, X., Zeng, S. and Xie, W. (2013) 'Nuclear receptors PXR and CAR: implications for drug metabolism regulation, pharmacogenomics and beyond', *Expert Opinion on Drug Metabolism & Toxicology*, 9(3), pp. 253–266. Available at: <https://doi.org/10.1517/17425255.2013.754010>.
- Ciemny, M., Kurcinski, M., Kamel, K., Kolinski, A., Alam, N., Schueler-Furman, O. and Kmiecik, S. (2018) 'Protein–peptide docking: opportunities and

- challenges', *Drug Discovery Today*, 23(8), pp. 1530–1537. Available at: <https://doi.org/10.1016/j.drudis.2018.05.006>.
- Dewi, P.P.P. (2019) 'Molecular Docking Terpinen-4-ol pada Protein IKK sebagai Antiinflamasi pada Aterosklerosis secara In Silico', *Jurnal Farmasi Udayana*, pp. 44. Available at: <https://doi.org/10.24843/JFU.2019.v08.i01.p07>.
- Dhianawaty, D., Nurfazriah, L.R. and Rezano, A. (2020) 'Gallic Acid Content and Antioxidant Activity of Pomegranate Peel Ethanol Extract', *Majalah Kedokteran Bandung*, 52(4). Available at: <https://doi.org/10.15395/mkb.v52n4.2108>.
- Elbarbry, F., Ung, A. and Abdelkawy, K. (2017) 'Studying the Inhibitory Effect of Quercetin and Thymoquinone on Human Cytochrome P450 Enzyme Activities', *Pharmacognosy Magazine*, 13(52), pp. 5.
- Fadhilah, A., Susanti, S. and Gultom, T. (2018a) 'Batu Village Deli Serdang, North Sumatera', pp. 11.
- 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), pp. 905–919. Available at: <https://doi.org/10.1038/nprot.2016.051>.
- Frimayanti, N., Zamri, A., Eryanti, Y., Herfindo, N. and Azteria, V. (2021) 'Docking and Molecular Dynamic Simulations Study to Search Curcumin Analogue Compounds as Potential Inhibitor Against SARS-CoV-2: A Computational Approach', *Jurnal Kimia Sains dan Aplikasi*, 24(3), pp. 85–90. Available at: <https://doi.org/10.14710/jksa.24.3.85-90>.
- Hirudkar, J.R., Parmar, K.M., Prasad, R.S., Sinha, S.K., Lomte, A.D., Itankar, P.R. and Prasad, S.K. (2020) 'The antidiarrhoeal evaluation of Psidium guajava L. against enteropathogenic Escherichia coli induced infectious diarrhoea', *Journal of Ethnopharmacology*, 251, pp. 112561. Available at: <https://doi.org/10.1016/j.jep.2020.112561>.
- Honkakoski, P. and Negishi, M. (2000) 'Regulation of cytochrome P450 (CYP) genes by nuclear receptors'.
- Ikawati, Zulies, (2018) 'Farmakologi Molekuler: Target Aksi Obat dan Mekanisme Molekulernya' Gajah Mada University Press, Yogyakarta.
- Jaghooori, M.M., Bleijlevens, B. and Olabarriaga, S.D. (2016) '1001 Ways to run AutoDock Vina for virtual screening', *Journal of Computer-Aided Molecular Design*, 30(3), pp. 237–249. Available at: <https://doi.org/10.1007/s10822-016-9900-9>.
- Jyrkkärinne, J., Windshügel, B., Mäkinen, J., Ylisirniö, M., Peräkylä, M., Poso, A., Sippl, W. and Honkakoski, P. (2005) 'Amino Acids Important for Ligand

- Specificity of the Human Constitutive Androstane Receptor', *Journal of Biological Chemistry*, 280(7), pp. 5960–5971. Available at: <https://doi.org/10.1074/jbc.M411241200>.
- Karlina, L. and Hafshah, M. (2019) 'Desain Turunan Kalkon Baru Sebagai Antikanker Payudara Berdasarkan Molecular Docking', *Walisongo Journal of Chemistry*, 2(2), pp. 57. Available at: <https://doi.org/10.21580/wjc.v2i2.6025>.
- Kumar, M., Tomar, M., Amarowicz, R., Saurabh, V., Nair, M.S., Maheshwari, C., Sasi, M., Prajapati, U., Hasan, M., Singh, S., Changan, S., Prajapat, R.K., Berwal, M.K. and Satankar, V. (2021) 'Guava (*Psidium guajava* L.) Leaves: Nutritional Composition, Phytochemical Profile, and Health-Promoting Bioactivities', *Foods*, 10(4), pp. 752. Available at: <https://doi.org/10.3390/foods10040752>.
- Lau, A.J. and Chang, T.K.H. (2015) '3-Hydroxyflavone and structural analogues differentially activate pregnane X receptor: Implication for inflammatory bowel disease', *Pharmacological Research*, 100, pp. 64–72. Available at: <https://doi.org/10.1016/j.phrs.2015.07.031>.
- Lelita, R., Gunawan, R. and Astuti, W. (2017) 'Studi Docking Molecular Swnyawa Kuersetin, Kalkon Dan Turunannya Sebagai Inhibitor Sel Kanker Payudara MC-7 (Michigan Cancer Foundation-7)'
- Li, L., Stanton, J.D., Tolson, A.H., Luo, Y. and Wang, H. (2009) 'Bioactive Terpenoids and Flavonoids from Ginkgo Biloba Extract Induce the Expression of Hepatic Drug-Metabolizing Enzymes Through Pregnane X Receptor, Constitutive Androstane Receptor, and Aryl hydrocarbon Receptor-Mediated Pathways', *Pharmaceutical Research*, 26(4), pp. 872–882. Available at: <https://doi.org/10.1007/s11095-008-9788-8>.
- Li, Z.-J., Guo, X., Dawuti, G. and Aibai, S. (2015) 'Antifungal Activity of Ellagic Acid *In Vitro* and *In Vivo*: Antifungal Activity Of Ellagic Acid *In Vitro* and *In Vivo*', *Phytotherapy Research*, 29(7), pp. 1019–1025. Available at: <https://doi.org/10.1002/ptr.5340>.
- Makatita, F.A. and Wardhani, R. (2020) 'Riset In Silico Dalam Pengembangan Sains Di Bidang Pendidikan, Studi Kasus: Analisis Potensi Cendana Sebagai Agen Anti-aging', pp. 9.
- Meng, X.-Y., Zhang, H.-X., Mezei, M. and Cui, M. (2011) 'Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery', *Current Computer Aided-Drug Design*, 7(2), pp. 146–157. Available at: <https://doi.org/10.2174/157340911795677602>.
- Morris, G.M. and Lim-Wilby, M. (2008) 'Molecular Docking', in A. Kukol (ed.) *Molecular Modeling of Proteins*. Totowa, NJ: Humana Press (Methods in

- Molecular Biology), pp. 365–382. Available at: https://doi.org/10.1007/978-1-59745-177-2_19.
- Mutoh, S., Sobhany, M., Moore, R., Perera, L., Pedersen, L., Sueyoshi, T. and Negishi, M. (2013) ‘Phenobarbital Indirectly Activates the Constitutive Active Androstane Receptor (CAR) by Inhibition of Epidermal Growth Factor Receptor Signaling’, *Science Signaling*, 6(274). Available at: <https://doi.org/10.1126/scisignal.2003705>.
- Nauli, T. (2014) ‘Penentuan Sisi Aktif Selulase *Aspergillus Niger* Dengan Docking Ligan’, *Jurnal Kimia Terapan Indonesia*, 16(2), pp. 94–100. Available at: <https://doi.org/10.14203/jkti.v16i2.14>.
- Niveshika, Verma, E., Maurya, S.K., Mishra, R. and Mishra, A.K. (2017) ‘The Combined Use of in Silico, in Vitro, and in Vivo Analyses to Assess Anti-cancerous Potential of a Bioactive Compound from Cyanobacterium *Nostoc* sp. MGL001’, *Frontiers in Pharmacology*, 8, pp. 873. Available at: <https://doi.org/10.3389/fphar.2017.00873>.
- Pantsar, T. and Poso, A. (2018) ‘Binding Affinity via Docking: Fact and Fiction’, *Molecules*, 23(8), pp. 1899. Available at: <https://doi.org/10.3390/molecules23081899>.
- Pinzi, L. and Rastelli, G. (2019) ‘Molecular Docking: Shifting Paradigms in Drug Discovery’, *International Journal of Molecular Sciences*, 20(18), pp. 4331. Available at: <https://doi.org/10.3390/ijms20184331>.
- Priyanga K, S. and K, V. (2017) ‘Investigation Of Antioxidant Potential Of Quercetin And Hesperidin: An In Vitro Aproach’, *Asian Journal of Pharmaceutical and Clinical Research*, 10(11), pp. 83. Available at: <https://doi.org/10.22159/ajpcr.2017.v10i11.20260>.
- Putri, Y.K. and Rusdiana, T. (2017) ‘Perbandingan Berbagai Interaksi Obat Dengan Herbal: Article Review’, 14, pp. 11.
- Rastinejad, F., Huang, P., Chandra, V. and Khorasanizadeh, S. (2013), ‘Understanding nuclear receptor form and function using structural biology’, *Journal of Molecular Endocrinology*, 51(3), pp. T1–T21. Available at: <https://doi.org/10.1530/JME-13-0173>.
- Rafdi, M.A. (2020), ‘Penambatan Molekuler senyawa turunan isoflavon sebagai penghambat protein tyrosine phosphatase-1B (PTP-1B)’, Skripsi, Fakultas Ilmu-Ilmu Kesehatan Universitas Jenderal Soedirman Purwokerto
- Sakurai, H., Suzuki, M., Itakura, S., Todo, H., Arce, F., See, G., Tanikawa, T. and Inoue, Y. (2022) ‘Preparation, Characterization, Solubility, and Antioxidant Capacity of Ellagic Acid-Urea Complex’, *Materials*, 15(8), pp. 2836. Available at: <https://doi.org/10.3390/ma15082836>.

- Sampath Kumar, N.S., Sarbon, N.M., Rana, S.S., Chintagunta, A.D., Prathibha, S., Ingilala, S.K., Jeevan Kumar, S.P., Sai Anvesh, B. and Dirisala, V.R. (2021) 'Extraction of bioactive compounds from Psidium guajava leaves and its utilization in preparation of jellies', *AMB Express*, 11(1), pp. 36. Available at: <https://doi.org/10.1186/s13568-021-01194-9>.
- Sari, I.W., Junaidin, J. and Pratiwi, D. (2020) 'Studi Molecular Docking Senyawa Flavonoid Herba Kumis Kucing (*Orthosiphon stamineus* B.) Pada Reseptor α -Glukosidase Sebagai Antidiabetes Tipe 2', *Jurnal Farmagazine*, 7(2), pp. 54. Available at: <https://doi.org/10.47653/farm.v7i2.194>.
- Sari, I.W. and Pratiwi, D. (2020) 'Molecular Docking Study Flavonoid Compounds From Kumir Kucing', pp. 7.
- Sarjit, A., Wang, Y. and Dykes, G.A. (2015) 'Antimicrobial activity of gallic acid against thermophilic *Campylobacter* is strain specific and associated with a loss of calcium ions', *Food Microbiology*, 46, pp. 227–233. Available at: <https://doi.org/10.1016/j.fm.2014.08.002>.
- Schäfer, A.M., Potterat, O., Seibert, I., Fertig, O. and Meyer zu Schwabedissen, H.E. (2019) 'Hyperforin-Induced Activation of the Pregnane X Receptor Is Influenced by the Organic Anion-Transporting Polypeptide 2B1', *Molecular Pharmacology*, 95(3), pp. 313–323. Available at: <https://doi.org/10.1124/mol.118.114066>.
- Setiawan, F.F. and Istyastono, E.P. (no date) 'Uji In Silico Senyawa 2,6-Dihidroksiantraquinon Sebagai Ligan Pada Reseptor Estrogen Alfa', pp. 4.
- Simbolon, R.A., Halimatussakdiah, H. and Amna, U. (2021) 'Uji Kandungan Senyawa Metabolit Sekunder pada Ekstrak Daun Jambu Biji (*Psidium guajava* L var. *Pomifera*) dari Kota Langsa, Aceh', *QUIMICA: Jurnal Kimia Sains dan Terapan*, 3(1), pp. 12–18. Available at: <https://doi.org/10.33059/jq.v3i1.3493>.
- Sundhani, E., Nugroho, A.E., Nurrochmad, A. and Lukitaningsih, E. (2022) 'Molecular interactions of *Andrographis paniculata* Burm. f. Active Compound with Nuclear Receptor (CAR and PXR): An In Silico Assessment Approach', *Indonesian Journal of Chemistry*, 22(1), pp. 126. Available at: <https://doi.org/10.22146/ijc.67981>.
- Suprijono, M., Sujuti, H., Kurnia, D., Widjanarko, S. (2020) 'Absorption, distribution, metabolism, excretion, and toxicity evaluation of Papua red fruit flavonoids through a computational study', ECS, doi : 10.1088/1755-1315/475/1/012078
- Tavares, W. de S., Martin-Pastor, M., Tavares, A.G. and Sousa, F.F.O. (2018) 'Biopharmaceutical Activities Related to Ellagic Acid, Chitosan, and Zein and Their Improvement by Association', *Journal of Food Science*, 83(12), pp. 2970–2975. Available at: <https://doi.org/10.1111/1750-3841.14369>.

- Wada, T., Gao, J. and Xie, W. (2009) 'PXR and CAR in energy metabolism', *Trends in Endocrinology & Metabolism*, 20(6), pp. 273–279. Available at: <https://doi.org/10.1016/j.tem.2009.03.003>.
- Wang, H., Faucette, S., Moore, R., Sueyoshi, T., Negishi, M. and LeCluyse, E. (2004) 'Human Constitutive Androstane Receptor Mediates Induction of CYP2B6 Gene Expression by Phenytoin', *Journal of Biological Chemistry*, 279(28), pp. 29295–29301. Available at: <https://doi.org/10.1074/jbc.M400580200>.
- Watkins, R.E., Maglich, J.M., Moore, L.B., Wisely, G.B., Noble, S.M., Davis-Searles, P.R., Lambert, M.H., Kliewer, S.A. and Redinbo, M.R. (2003) '2.1 Å Crystal Structure of Human PXR in Complex with the St. John's Wort Compound Hyperforin', *Biochemistry*, 42(6), pp. 1430–1438. Available at: <https://doi.org/10.1021/bi0268753>.
- Warnasih, S., Ishlah, T., Novitasari, Azzahra, D., Syahputra, G. (2022) 'Aktivitas Imunostimulan Ekstrak Metanol Biji Kurma (Phoenix dactylifera) secara In Silico terhadap Reseptor GIF dan COX-2 serta Uji In Vitro melalui Proliferasi Sel Limfosit Mencit', 10(2), pp. 48-59.
- Willson, T.M. and Kliewer, S.A. (2002) 'Pxr, car and drug metabolism', *Nature Reviews Drug Discovery*, 1(4), pp. 259–266. Available at: <https://doi.org/10.1038/nrd753>.
- Yi Shu (2011) 'Antibacterial activity of quercetin on oral infectious pathogens', *African Journal of Microbiology Research*, 5(30). Available at: <https://doi.org/10.5897/AJMR11.849>.
- Zanger, U.M. and Klein, K. (2013) 'Pharmacogenetics of cytochrome P450 2B6 (CYP2B6): advances on polymorphisms, mechanisms, and clinical relevance', *Frontiers in Genetics*, 4. Available at: <https://doi.org/10.3389/fgene.2013.00024>.