

## DAFTAR PUSTAKA

- Agaatsz, J.N. and Sitompul, M. (2021) *View of Tingkat Pengetahuan dan Sikap Orangtua Berhubungan dengan Penggunaan Obat Tradisional pada Anak, Jurnal Penelitian Perawat Profesional.* Available at: <https://doi.org/https://doi.org/10.37287/jppp.v3i2.454>.
- Ahmad, A., Husain, A., Mujeeb, M., Khan, S.A., Najmi, A.K., Siddique, N.A., Damanhour, Z.A. and Anwar, F. (2013) ‘A Review on Therapeutic Potential of *Nigella Sativa*: A Miracle Herb’, *Asian Pacific Journal of Tropical Biomedicine*, 3(5), pp. 337–352. Available at: [https://doi.org/10.1016/S2221-1691\(13\)60075-1](https://doi.org/10.1016/S2221-1691(13)60075-1).
- Albassam, A.A., Ahad, A., Alsultan, A. and Al-Jenoobi, F.I. (2018) ‘Inhibition of Cytochrome P450 Enzymes by Thymoquinone in Human Liver Microsomes’, *Saudi Pharmaceutical Journal*, 26(5), pp. 673–677. Available at: <https://doi.org/10.1016/j.jps.2018.02.024>.
- Al-Khalifa, K.S., Alsheikh, R., Al-Hariri, M.T., El-Sayyad, H., Alqurashi, M.S., Ali, S. and Bugshan, A.S. (2021) ‘Evaluation of the Antimicrobial Effect of Thymoquinone Against Different Dental Pathogens: An *in vitro* study’, *Molecules*, 26(21). Available at: <https://doi.org/10.3390/molecules26216451>.
- Almshawit, H. and Macreadie, I. (2017) ‘Fungicidal Effect of Thymoquinone Involves Generation of Oxidative Stress in *Candida glabrata*’, *Microbiological Research*, 195, pp. 81–88. Available at: <https://doi.org/10.1016/j.micres.2016.11.008>.
- 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. 1219–1224. Available at: <https://doi.org/10.5958/0976-5506.2019.01752.2>.
- Bai, Q., Li, L., Liu, S., Xiao, S., Guo, Y. and Author, C. (2018) *Drug Design Progress of In Silico, In Vitro and In Vivo Researches.* Available at: [www.proteinmodelportal.org](http://www.proteinmodelportal.org).

- Banerjee, M., Robbins, D. and Chen, T. (2015) 'Targeting Xenobiotic Receptors PXR and CAR in Human Diseases', *Drug Discovery Today*. Elsevier Ltd, pp. 618–628. Available at: <https://doi.org/10.1016/j.drudis.2014.11.011>.
- Bock, K.W. and Kohle, C. (2004) 'Coordinate Regulation of Drug Metabolism by Xenobiotic Nuclear Receptors: UGTs Acting Together With CYPs and Glucuronide Transporters', *Drug Metabolism Reviews*, pp. 595–615. Available at: <https://doi.org/10.1081/DMR-200033455>.
- Brilhante, R.S.N., Caetano, É.P., Lima, R.A.C. de, Marques, F.J. de F., Castelo-Branco, D. de S.C.M., Melo, C.V.S. de, Guedes, G.M. de M., Oliveira, J.S. de, Camargo, Z.P. de, Moreira, J.L.B., Monteiro, A.J., Bandeira, T. de J.P.G., Cordeiro, R. de A., Rocha, M.F.G. and Sidrim, J.J.C. (2016) 'Terpinen-4-ol, Tyrosol, and β-lapachone as Potential Antifungals Against Dimorphic Fungi', *Brazilian Journal of Microbiology*, 47(4), pp. 917–924. Available at: <https://doi.org/10.1016/j.bjm.2016.07.015>.
- 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 and Toxicology*. Taylor and Francis Ltd, pp. 635–647. Available at: <https://doi.org/10.1080/17425255.2018.1476488>.
- Chaieb, K., Kouidhi, B., Jrah, H., Mahdouani, K. and Bakhrouf, A. (2011) 'Antibacterial Activity of Thymoquinone, an Active Principle of *Nigella Sativa* and its Potency to Prevent Bacterial Biofilm Formation', *BMC Complementary and Alternative Medicine*, 11. Available at: <https://doi.org/10.1186/1472-6882-11-29>.
- Cosconati, S., Forli, S., Perryman, A.L., Harris, R., Goodsell, D.S. and Olson, A.J. (2010) 'Virtual Screening with AutoDock: Theory and Practice', *Expert Opinion on Drug Discovery*, pp. 597–607. Available at: <https://doi.org/10.1517/17460441.2010.484460>.
- El-Dakhakhny, M., Madi, N.J., Lembert, N. and Ammon, H.P.T. (2002) *Nigella Sativa Oil, Nigellone and Derived Thymoquinone Inhibit Synthesis of 5-Lipoxygenase Products in Polymorphonuclear Leukocytes from Rats*. Available at: [www.elsevier.com/locate/jethpharm](http://www.elsevier.com/locate/jethpharm).

- Elsharkawy, E.R., Abdallah, E.M. and Markb, A.A. (2021) *Potential Cytotoxic, Antifungal, and Antioxidant Activity of Dithymoquinone and Thymoquinone.*
- Ferreira, L.G., dos Santos, R.N., Oliva, G. and Andricopulo, A.D. (2015) ‘Molecular Docking and Structure-Based Drug Design Strategies’, *Molecules*. MDPI AG, pp. 13384–13421. Available at: <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), pp. 905–919. Available at: <https://doi.org/10.1038/nprot.2016.051>.
- Germain, P., Altucci, L., Bourguet, W., Rochette-Egly, C. and Gronemeyer, H. (2003) *Topic 1.1 Nuclear receptor superfamily: Principles of signaling, Pure Appl. Chem.* Available at: <http://www.ens-lyon.fr/LBMC/LAUDET/nomenc.html>.
- Hanif, A.U., Lukis, P.A. and Fadlan, A. (2020) ‘Pengaruh Minimisasi Energi MMFF94 dengan MarvinSketch dan Open Babel PyRx pada Penambatan Molekular Turunan Oksindola Tersubstitusi’, *ALCHEMY:Journal of Chemistry*, 8(2), pp. 33–40. Available at: <https://ejurnal.uin-malang.ac.id/index.php/Kimia/article/view/10481> (Accessed: 9 March 2023).
- Hannan, M.A., Rahman, M.A., Sohag, A.A.M., Uddin, M.J., Dash, R., Sikder, M.H., Rahman, M.S., Timalsina, B., Munni, Y.A., Sarker, P.P., Alam, M., Mohibullah, M., Haque, M.N., Jahan, I., Hossain, M.T., Afrin, T., Rahman, M.M., Tahjib-Ul-arif, M., Mitra, S., Oktaviani, D.F., Khan, M.K., Choi, H.J., Moon, I.S. and Kim, B. (2021) ‘Black cumin (*Nigella Sativa* L.): A Comprehensive Review on Phytochemistry, Health Benefits, Molecular Pharmacology, and Safety’, *Nutrients*. MDPI AG. Available at: <https://doi.org/10.3390/nu13061784>.
- Jukic, M., Politeo, O., Maksimovic, M., Milos, Mia and Milos, Mladen (2007) ‘*In Vitro* Acetylcholinesterase Inhibitory Properties of Thymol, Carvacrol and

- their Derivatives Thymoquinone and Thymohydroquinone', *Phytother. Res.*, 21(21), pp. 259–261. Available at: <https://doi.org/10.1002/ptr>.
- 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', *The Journal of biological chemistry*, 280(7), pp. 5960–5971. Available at: <https://doi.org/10.1074/JBC.M411241200>.
- Kamaraj, R., Drastik, M., Maixnerova, J. and Pavek, P. (2022) 'Allosteric Antagonism of the Pregnan X Receptor (PXR): Current-State-of-the-Art and Prediction of Novel Allosteric Sites', *Cells*, 11(19). Available at: <https://doi.org/10.3390/CELLS11192974>.
- Kolina, J., Sumiwi, S.A. and Levita, J. (2019) 'Mode Ikatan Metabolit Sekunder Di Tanaman Akar Kuning (*Arcangelisia flava* L.) Dengan Nitrat Oksida Sintase', *FITOFARMAKA: Jurnal Ilmiah Farmasi*, 8(1), pp. 45–52. Available at: <https://doi.org/10.33751/jf.v8i1.1171>.
- Lau, A.J. and Chang, T.K.H. (2015) '3-Hydroxyflavone and Structural Analogs Differentially Activate Pregnan 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>.
- Lima, M.D.S., Quintans-Júnior, L.J., de Santana, W.A., Martins Kaneto, C., Pereira Soares, M.B. and Villarreal, C.F. (2013) 'Anti-Inflammatory Effects of Carvacrol: Evidence for a Key Role of Interleukin-10', *European Journal of Pharmacology*, 699(1–3), pp. 112–117. Available at: <https://doi.org/10.1016/j.ejphar.2012.11.040>.
- Liu, Y.H., Mo, S.L., Bi, H.C., Hu, B.F., Li, C.G., Wang, Y.T., Huang, L., Huang, M., Duan, W., Liu, J.P., Wei, M.Q. and Zhou, S.F. (2011) 'Regulation of Human Pregnan X Receptor and its Target Gene Cytochrome P450 3A4 by Chinese Herbal Compounds and a Molecular Docking Study', *Xenobiotica*, 41(4), pp. 259–280. Available at: <https://doi.org/10.3109/00498254.2010.537395>.
- Mahfur, M. (2018) 'Profil Metabolit Sekunder Senyawa Aktif Minyak Atsiri Jinten Hitam (*Nigella sativa* L.) dari Habasyah dan India', *PHARMACY: Jurnal*

- Farmasi Indonesia (Pharmaceutical Journal of Indonesia)*, 15(1), pp. 90–97. Available at: <http://jurnahnasional.ump.ac.id/index.php/PHARMACY/article/view/2274> (Accessed: 29 October 2022).
- Manna, A., Laksitorini, M.D., Hudiyanti, D. and Siahaan, P. (2017) ‘Molecular Docking of Interaction between E-Cadherin Protein and Conformational Structure of Cyclic Peptide ADTC3 (Ac-CADTPC-NH2) Simulated on 20 ns’, *Jurnal Kimia Sains dan Aplikasi*, 20(1), pp. 30–36. Available at: <https://doi.org/10.14710/JKSA.20.1.30-36>.
- Marlinda, L. (2015) *Effectivity Of Black Cumin Seeds Extract To Increase Phagocytosis, J MAJORITY /.*
- Meng, X.-Y., Zhang, H.-X., Mezei, M. and Cui, M. (2012) *Molecular Docking: A Powerful Approach For Structure-Based Drug Discovery*.
- Muttaqin, F.Z., Ismail, H. and Muhammad, H.N. (2019) ‘Studi Molecular Docking, Molecular Dynamic, Dan Prediksi Toksisitas Senyawa Turunan Alkaloid Naftiridin Sebagai Inhibitor Protein Kasein Kinase 2- $\alpha$  Pada Kanker Leukemia’, *Pharmacoscript*, 2(2), pp. 131–151. Available at: <https://doi.org/10.36423/PHARMACOSCRIPT.V2I2.241>.
- Nauli, T. and 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>.
- Ningtyas, E.A.E. (2015) ‘Aktivasi Pemakaian Jinten Hitam (*Nigella sativa*) Terhadap Respons Imun Pada Gigi yang MengalamiInflamasi’, *STOMATOGNATIC - Jurnal Kedokteran Gigi*, 9(1), pp. 48–53. Available at: <https://jurnal.unej.ac.id/index.php/STOMA/article/view/2105> (Accessed: 8 February 2023).
- Nogueira, M.N.M., Aquino, S.G., Rossa, C. and Spolidorio, D.M.P. (2014) ‘Terpinen-4-ol and Alpha-Terpineol (Tea Tree Oil Components) Inhibit the Production of IL-1 $\beta$ , IL-6 and IL-10 on Human Macrophages’, *Inflammation Research*, 63(9), pp. 769–778. Available at: <https://doi.org/10.1007/s00011-014-0749-x>.
- Nyemb, J.N., Shaheen, H., Wasef, L., Nyamota, R., Segueni, N. and El-Saber Batiha, G. (2022) ‘Black Cumin: A Review of its Pharmacological Effects

- and its Main Active Constituent', *Pharmacognosy Reviews*, 16(32), pp. 107–125. Available at: <https://doi.org/10.5530/phrev.2022.16.16>.
- Pantsar, T. and Poso, A. (2018) 'Binding Affinity via Docking: Fact and Fiction', *Molecules*, 23(8), pp. 1–11. Available at: <https://doi.org/10.3390/MOLECULES23081899>.
- 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 Leads the Pathways of Drug-Designing', *PLoS ONE*, 5(8), pp. 1–10. Available at: <https://doi.org/10.1371/journal.pone.0012029>.
- Prasetiawati, R., Suherman, M., Permana, B. and Rahmawati, R. (2021) 'Molecular Docking Study of Anthocyanidin Compounds Against Epidermal Growth Factor Receptor (EGFR) as Anti-Lung Cancer', *Indonesian Journal of Pharmaceutical Science and Technology*, 8(1), pp. 8–20. Available at: <https://doi.org/10.24198/IJPST.V8I1.29872>.
- Prayoga, harry, Yulianti, Y. and Riyanto, A. (2018) 'Analisis Dinamika Molekul Protein Lysozyme Putih Telur dengan Model Potensial Lennard-Jones Menggunakan Aplikasi Gromacs', *Jurnal Teori dan Aplikasi Fisika*, 6(2), pp. 239–248. Available at: <https://doi.org/10.23960/JTAF.V6I2.1849>.
- Rachmania, R.A., Supandi and Cristina, F.A.D. (2016) 'Analisis Penambatan Molekul Senyawa Flavonoid Buah Mahkota Dewa (Phaleria macrocarpa (Scheff.) Boerl.) Pada Reseptor  $\alpha$ -Glukosidase Sebagai Antidiabetes', *Pharmaceutical Journal of Indonesia*, 13(2), pp. 239–251.
- Riverson, M. and Rizarullah (2020) 'Potensi Antidiabetes Benzyl Beta D Glucopyranoside Dari Daun Yacon Sebagai Inhibitor Enzim DPP-4: Metode In Silico', *Prosiding Seminar Nasional Biotik*, 8(1), pp. 300–305. Available at: <https://doi.org/10.22373/pbio.v8i2.9653>.
- 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*, 4(1), pp. 16–20. Available at: <https://doi.org/10.24198/CNA.V4.N1.10443>.

- Sari, I.W., Junaidin and Pratiwi, D. (2020) ‘Studi Molecular Docking Senyawa Flavonoid Herba Kumis Kucing (*Orthosiphon Stamineus B.*) pada Reseptor  $\alpha$ -Glukosidase sebagai Antidiabetes Tipe 2’, *Jurnal Farmagazine*, 7(2), pp. 54–60. Available at: <https://doi.org/10.47653/FARM.V7I2.194>.
- Sarkar, C., Jamaddar, S., Islam, T., Mondal, M., Islam, M.T. and Mubarak, M.S. (2021) ‘Therapeutic Perspectives of the Black Cumin Component Thymoquinone: A Review’, *Food and Function*. Royal Society of Chemistry, pp. 6167–6213. Available at: <https://doi.org/10.1039/d1fo00401h>.
- Sastray, G.M., Adzhigirey, M., Day, T., Annabhimoju, R. and Sherman, W. (2013) ‘Protein And Ligand Preparation: Parameters, Protocols, And Influence On Virtual Screening Enrichments’, *Journal of computer-aided molecular design*, 27(3), pp. 221–234. Available at: <https://doi.org/10.1007/S10822-013-9644-8>.
- Shivanika, C., Deepak Kumar, S., Ragunathan, V., Tiwari, P., Sumitha, A. and Brindha Devi, P. (2022) ‘Molecular Docking, Validation, Dynamics Simulations, and Pharmacokinetic Prediction of Natural Compounds Against the SARS-CoV-2 Main-Protease’, *Journal of Biomolecular Structure and Dynamics*, 40(2), pp. 585–611. Available at: <https://doi.org/10.1080/07391102.2020.1815584>.
- Shofi, M. (2021) *Analisis Senyawa  $\alpha$ -spinasterol Pada Biji Trembesi (Samanea saman (jacq.) Merr) Terhadap Penghambatan 3C-like Protease SARS-CoV-2 Melalui Uji In Silico*, *Jurnal Sintesis*. Available at: <http://eprints.iik.ac.id/id/eprint/30/> (Accessed: 25 March 2023).
- Suciayati, A.N., Nurcahyani, N., Rosa Jurusan Biologi Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Lampung Jl Soemantri Brodjonegoro, E. and Lampung, B. (2020) ‘The Effect of Black Jintan Extract (*Nigella sativa*) Towards The Fetus Bone Structure from Mencit (*Mus musculus L.*)’, *Jurnal Ilmiah Biologi Eksperimen dan Keanekaragaman Hayati*, 7(1), pp. 40–46.
- Suhadi, A., Rizarullah, R. and Feriyani, F. (2019) ‘Simulasi Docking Senyawa Aktif Daun Binahong Sebagai Inhibitor Enzyme Aldose Reductase’, *Sel*

- Jurnal Penelitian Kesehatan*, 6(2), pp. 55–65. Available at: <https://doi.org/10.22435/SEL.V6I2.1651>.
- 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. 126–141. Available at: <https://doi.org/10.22146/ijc.67981>.
- Susanti, N.M.P., Laksmani, N.P.L., Noviyanti, N.K.M., Arianti, K.M. and Duantara, I.K. (2019) ‘Molecular Docking Terpinen-4-ol Sebagai Antiinflamasi Pada Aterosklerosis Secara In Silico’, *Jurnal Kimia (Juournal Of Chemistry)*, 13(2), pp. 221–228. Available at: <https://doi.org/10.24843/jchem.2019.v13.i02.p16>.
- Syahputra, G., Ambarsari, L. and Sumaryada, T. (2014) ‘Simulasi Docking Kurkumin Enol. Bisdemetoksikurkumin dan Analognya Sebagai Inhibitor Enzim12-Lipoksgigenase’, *Jurnal Biofisika*, 10(1), pp. 55–67. Available at: <https://journal.ipb.ac.id/index.php/biofisika/article/view/9354> (Accessed: 25 March 2023).
- Trevisan, D.A.C., da Silva, A.F., Negri, M., de Abreu Filho, B.A., Machinski Junior, M., Patussi, E.V., Campanerut-Sá, P.A.Z. and Mikcha, J.M.G. (2018) ‘Antibacterial and Antibiofilm Activity of Carvacrol Against *Salmonella enterica* serotype *typhimurium*’, *Brazilian Journal of Pharmaceutical Sciences*, 54(1). Available at: <https://doi.org/10.1590/s2175-97902018000117229>.
- 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>.
- Wallace, B.D. and Redinbo, M.R. (2013) ‘Xenobiotic-Sensing Nuclear Receptors Involved in Drug Metabolism: A Structural Perspective’, *Drug Metabolism Reviews*, pp. 79–100. Available at: <https://doi.org/10.3109/03602532.2012.740049>.

- 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>.
- Xie, G., Chen, N., Soromou, L.W., Liu, F., Xiong, Y., Wu, Q., Li, H., Feng, H. and Liu, G. (2012) 'p-Cymene Protects Mice Against Lipopolysaccharide-Induced Acute Lung Injury by Inhibiting Inflammatory Cell Activation', *Molecules*, 17(7), pp. 8159–8173. Available at: <https://doi.org/10.3390/molecules17078159>.
- Yasin, S.A., Azzahra, A., Ramadhan, N.E. and Mylanda, V. (2020) 'Studi Penambatan Molekuler dan Prediksi ADMET Senyawa Bioaktif Beberapa Jamu Indonesia terhadap SARS-CoV-2 Main Protease (Mpro)', *Berkala Ilmiah Mahasiswa Farmasi Indonesia*, 7(2), pp. 24–41. Available at: <https://doi.org/10.48177/BIMFI.V7I2.45>.
- Zhong, W., Chi, G., Jiang, L., Soromou, L.W., Chen, N., Huo, M., Guo, W., Deng, X. and Feng, H. (2013) 'p-Cymene Modulates In Vitro And In Vivo Cytokine Production by Inhibiting MAPK and NF-κB Activation', *Inflammation*, 36(3), pp. 529–537. Available at: <https://doi.org/10.1007/s10753-012-9574-y>.