# DAFTAR PUSTAKA

Abbott, D.H., Barnett, D.K., Bruns, C.M., dan Dumesic, D.A., 2005. Androgen excess fetal programming of female reproduction: a developmental aetiology for polycystic ovary syndrome? *Human Reproduction Update*, **11**: 357–374.

Abdulfatai, U., Uzairu, A., dan Uba, S., 2017. Quantitative structure-activity relationship and molecular docking studies of a series of quinazolinonyl analogues as inhibitors of gamma amino butyric acid aminotransferase. *Journal of Advanced Research*, **8**: 33–43.

Agarwal, S. dan Mehrotra, R., 2016. 'An overview of Molecular Docking', . URL: https://www.semanticscholar.org/paper/An-overview-of-Molecular-Docking-Agarwal-Mehrotra/e5621a1266f4967cf5db297bb18f982224831406 (diakses tanggal 11/12/2021).

Ahmed, S.M., Swamy, V., Gopkumar, P., dan Dhanapal, R., 2005. Anti-Diabetic Activity of Terminalia catappa Linn. Leaf Extracts in Alloxan-Induced Diabetic Rats. *Iranian Journal of Pharmacology and Therapeutics*, **4**: 36–0.

Alchetron, 2017. 'Terminalia catappa - Alchetron, The Free Social Encyclopedia', *Alchetron.com*. URL: https://alchetron.com/Terminalia-catappa (diakses tanggal 4/7/2022).

Al-Eisa, E., Gabr, S.A., dan Alghadir, A.H., 2017. Effects of supervised aerobic training on the levels of anti-Mullerian hormone and adiposity measures in women with normo-ovulatory and polycystic ovary syndrome. *JPMA. The Journal of the Pakistan Medical Association*, **67**: 499–507.

Anand, A.V., Divya, N., dan Kotti, P.P., 2015. An updated review of Terminalia catappa. *Pharmacognosy Reviews*, **9**: 93–98.

Ashraf, S., Nabi, M., Rasool, S. ul A., Rashid, F., dan Amin, S., 2019. Hyperandrogenism in polycystic ovarian syndrome and role of CYP gene variants: a review. *Egyptian Journal of Medical Human Genetics*, **20**: 25.

Azziz, R., 2008. Polycystic Ovary Syndrome Is a Family Affair. *The Journal of Clinical Endocrinology and Metabolism*, **93**: 1579–1581.

Azziz, R., Carmina, E., Dewailly, D., Diamanti-Kandarakis, E., Escobar-Morreale, H.F., Futterweit, W., dkk., 2006. Positions statement: criteria for defining polycystic ovary syndrome as a predominantly hyperandrogenic syndrome: an Androgen Excess Society guideline. *The Journal of Clinical Endocrinology and Metabolism*, **91**: 4237–4245.

Bachanek, M., Abdalla, N., Cendrowski, K., dan Sawicki, W., 2015. Value of ultrasonography in the diagnosis of polycystic ovary syndrome - literature review. *Journal of Ultrasonography*, **15**: 410–422.

Baptiste, C.G., Battista, M.-C., Trottier, A., dan Baillargeon, J.-P., 2010. Insulin and hyperandrogenism in women with polycystic ovary syndrome. *The Journal of Steroid Biochemistry and Molecular Biology*, **122**: 42–52.

Barbosa, G., Sá, L.B.P.C. de, Rocha, D.R.T.W., dan Arbex, A.K., 2016. Polycystic Ovary Syndrome (PCOS) and Fertility. *Open Journal of Endocrine and Metabolic Diseases*, **6**: 58–65.

Bashir, A., Guha, L., dan Bhat, I., 2021. Comprehension, Management, and Treatment of Polycystic Ovarian Syndrome via Allopathic, Unani and Ayurvedic Perspectives. *Clinical Journal of Woman s Health*, **21**: .

Berman, H.M., Kleywegt, G.J., Nakamura, H., dan Markley, J.L., 2013. The future of the Protein Data Bank. *Biopolymers*, **99**: 218–222.

Berman, H.M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T.N., Weissig, H., dkk., 2000. The Protein Data Bank. *Nucleic Acids Research*, **28**: 235–242.

Brown, S.H. dan Cooprider, K., 2013. Terminalia catappa, Department of Agriculture, Cooperative Extension Service, University of Florida, IFAS, Lee County Extension, Florida.

Burley, S.K., Bhikadiya, C., Bi, C., Bittrich, S., Chen, L., Crichlow, G.V., dkk., 2021. RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. *Nucleic Acids Research*, **49**: D437–D451.

Carvalho, L., Reis, F., Candido, A., Nunes, F., Ferreira, C., dan Gomes, K., 2018. Polycystic Ovary Syndrome as a systemic disease with multiple molecular pathways: A narrative review. *Endocrine Regulations*, **52**: 208–221.

Chandrasekhar, Y., Ramya, E.M., Navya, K., Phani Kumar, G., dan Anilakumar, K.R., 2017. Antidepressant like effects of hydrolysable tanins of Terminalia catappa leaf extract via modulation of hippocampal plasticity and regulation of monoamine neurotransmitters subjected to chronic mild stress (CMS). *Biomedicine & Pharmacotherapy = Biomedecine & Pharmacotherapie*, **86**: 414–425.

Chen, P.-S., Li, J.-H., Liu, T.-Y., dan Lin, T.-C., 2000. Folk medicine Terminalia catappa and its major tanin component, punicalagin, are effective against bleomycin-induced genotoxicity in Chinese hamster ovary cells. *Cancer Letters*, **152**: 115–122.

Chhabra, S., McCartney, C.R., Yoo, R.Y., Eagleson, C.A., Chang, R.J., dan Marshall, J.C., 2005. Progesterone inhibition of the hypothalamic gonadotropin-releasing hormone pulse generator: evidence for varied effects in hyperandrogenemic adolescent girls. *The Journal of Clinical Endocrinology and Metabolism*, **90**: 2810–2815.

Choudhary, P., Sevatkar, B., Sharma, S., dan Godatwar, P.K., 2020. Management of dermatological manifestation of PCOS by Pathadi and Kanchnaradi kwatha along with Arogyavardhini vati. *Asian Journal of Pharmaceutical Research*, **10**: 17–22.

Cornell, W.D., Cieplak, P., Bayly, C.I., Gould, I.R., Merz, K.M., Ferguson, D.M., dkk., 2002. 'A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules', *ACS Publications*. URL: https://pubs.acs.org/doi/pdf/10.1021/ja00124a002 (diakses tanggal 29/11/2021).

Dar, A.M. dan Mir, S., 2017. Molecular Docking: Approaches, Types, Applications and Basic Challenges. *Journal of Analytical & Bioanalytical Techniques*, **08**: .

Davies, M., Nowotka, M., Papadatos, G., Dedman, N., Gaulton, A., Atkinson, F., dkk., 2015. ChEMBL web services: streamlining access to drug discovery data and utilities. *Nucleic Acids Research*, **43**: W612–W620.

Dean, M., Austin, J., Jinhong, R., Johnson, M.E., Lantvit, D.D., dan Burdette, J.E., 2018. The Flavonoid Apigenin is a Progesterone Receptor Modulator with In Vivo Activity in the Uterus. *Hormones & cancer*, **9**: 265–277.

Denisov, I.G., Makris, T.M., Sligar, S.G., dan Schlichting, I., 2005. Structure and chemistry of cytochrome P450. *Chemical Reviews*, **105**: 2253–2277.

Deswal, R., Narwal, V., Dang, A., dan Pundir, C.S., 2020. The Prevalence of Polycystic Ovary Syndrome: A Brief Systematic Review. *Journal of Human Reproductive Sciences*, **13**: 261–271.

Devi, R., Sathya, S., dan Coumar, M., 2015. Evolutionary algorithms for de novo drug design – A survey. *Applied Soft Computing*, **27**: 543–552.

DiPiro, J.T., Talbert, R.L., Yee, G.C., Matzke, G.R., Wells, B.G., dan Posey, L.M., 2008. *Pharmacotherapy: A Pathophysiologic Approach*, 8th ed. Mc-Graw Hill Company.

Divya, N. dan Vijaya, A., 2014. Phytochemical investigation and in vitro anti-diabetic activity of Terminalia Catappa leaves. *International Journal of Phytopharmacy*, **4**: 132–134.

Du, Q.-S., Wang, Q.-Y., Du, L.-Q., Chen, D., dan Huang, R.-B., 2013. Theoretical study on the polar hydrogen-π (Hp-π) interactions between protein side chains. *Chemistry Central Journal*, **7**: 92.

Dutta, D., Bhattacharya, S., Khandelwal, D., Aggarwal, S., Singla, R., Surana, V., dkk., 2020. Clinical Practice Patterns of Polycystic Ovary Syndrome Among Doctors of Different Specialties—An Indian Perspective.

Eagleson, C.A., Gingrich, M.B., Pastor, C.L., Arora, T.K., Burt, C.M., Evans, W.S., dkk., 2000. Polycystic ovarian syndrome: evidence that flutamide restores sensitivity of the gonadotropin-releasing hormone pulse generator to inhibition by estradiol and progesterone. *The Journal of Clinical Endocrinology and Metabolism*, **85**: 4047–4052.

Eisen, M.B., Wiley, D.C., Karplus, M., dan Hubbard, R.E., 1994. HOOK: a program for finding novel molecular architectures that satisfy the chemical and steric requirements of a macromolecule binding site. *Proteins*, **19**: 199–221.

Fahmy, N.M., Al-Sayed, E., Abdel-Daim, M.M., Karonen, M., dan Singab, A.N., 2016. Protective effect of Terminalia muelleri against carbon tetrachloride-induced hepato and nephro-toxicity in mice and characterization of its bioactive constituents. *Pharmaceutical Biology*, **54**: 303–313.

Fauser, B.C.J.M., Tarlatzis, B.C., Rebar, R.W., Legro, R.S., Balen, A.H., Lobo, R., dkk., 2012. Consensus on women's health aspects of polycystic ovary syndrome (PCOS): the Amsterdam ESHRE/ASRM-Sponsored 3rd PCOS Consensus Workshop Group. *Fertility and Sterility*, **97**: 28-38.e25.

Ferreira, L.G., Dos Santos, R.N., Oliva, G., dan Andricopulo, A.D., 2015. Molecular docking and structure-based drug design strategies. *Molecules (Basel, Switzerland)*, **20**: 13384–13421.

Gao, J., Tang, X., Dou, H., Fan, Y., Zhao, X., dan Xu, Q., 2004. Hepatoprotective activity of Terminalia catappa L. leaves and its two triterpenoids. *The Journal of Pharmacy and Pharmacology*, **56**: 1449–1455.

Gay, S.C., Roberts, A.G., dan Halpert, J.R., 2010. Structural Features of Cytochromes P450 and Ligands that Affect Drug Metabolism as Revealed by X-ray Crystallography and NMR. *Future medicinal chemistry*, **2**: 1451–1468.

Gilling-Smith, C., Story, H., Rogers, V., dan Franks, S., 1997. Evidence for a primary abnormality of thecal cell steroidogenesis in the polycystic ovary syndrome. *Clinical Endocrinology*, **47**: 93–99.

Gilling-Smith, C., Willis, D.S., Beard, R.W., dan Franks, S., 1994. Hypersecretion of androstenedione by isolated thecal cells from polycystic ovaries. *The Journal of Clinical Endocrinology and Metabolism*, **79**: 1158–1165.

Häggström, M. dan Richfield, D., 2014. Diagram of the pathways of human steroidogenesis. *Wikiversity Journal of Medicine*, **1**: .

Haltje, H.-D., Sippl, W., Rognan, D., dan Folkers, G., 2008. *Molecular Modeling: Basic Principles and Applications*, 3rd edition. ed. Wiley-VCH, Weinheim.

Heyne, 1987. *Tumbuhan Berguna Indonesia*, 3rd ed. Departemen Kehutanan RI, Jakarta.

HIFERI, 2013. *Konsensus Penanganan Infertilitas*. Himpunan Endokrinologi Reproduksi dan Fertilitas Indonesia, Jakarta.

Hnawia, E., Hassani, L., Deharo, E., Maurel, S., Waikedre, J., Cabalion, P., dkk., 2011. Antiplasmodial activity of New Caledonia and Vanuatu traditional medicines. *Pharmaceutical Biology*, **49**: 369–376.

Hou, T. dan Xu, X., 2004. Recent development and application of virtual screening in drug discovery: an overview. *Current Pharmaceutical Design*, **10**: 1011–1033.

Hu, Q. dan Hartmann, R.W., 2014. Chapter 11 - The Renaissance of CYP17 Inhibitors for the Treatment of Prostate Cancer, dalam: Neidle, S. (Editor), *Cancer Drug Design and Discovery (Second Edition)*. Academic Press, San Diego, hal. 319–356.

Idemudia, O.G., 1970. Terpenoids of Nigerian Terminalia species. *Phytochemistry*, **9**: 2401–2.

Joham, A.E., Teede, H.J., Ranasinha, S., Zoungas, S., dan Boyle, J., 2015. Prevalence of infertility and use of fertility treatment in women with polycystic ovary syndrome: data from a large community-based cohort study. *Journal of Women's Health (2002)*, **24**: 299–307.

Kamboj, A., Verma, D., Sharma, D., Pant, K., Pant, B., dan Kumar, V., 2019. A Molecular Docking Study towards Finding Herbal Treatment against Polycystic Ovary Syndrome (PCOS) 2277–3878.

Kementerian Kesehatan RI, 2013. Riset Kesehatan Dasar 2013.

Khan, M.J., Ullah, A., dan Basit, S., 2019. Genetic Basis of Polycystic Ovary Syndrome (PCOS): Current Perspectives. *The Application of Clinical Genetics*, **12**: 249–260.

Kitchen, D.B., Decornez, H., Furr, J.R., dan Bajorath, J., 2004. Docking and scoring in virtual screening for drug discovery: methods and applications. *Nature Reviews. Drug Discovery*, **3**: 935–949.

Kleywegt, G.J., 2000. Validation of protein crystal structures. *Acta Crystallographica Section D Biological Crystallography*, **56**: 249–265.

Kooistra, A.J., Mordalski, S., Pándy-Szekeres, G., Esguerra, M., Mamyrbekov, A., Munk, C., dkk., 2021. GPCRdb in 2021: integrating GPCR sequence, structure and function. *Nucleic Acids Research*, **49**: D335–D343.

Kurobe, F.M.C., Dzik, A., Cavagna, M., dan Drezett, J., 2012. Importância do hormônio anti-Mülleriano na infertilidade. *Reprodução & Climatério*, **27**: 104–108.

Legro, R., 2015. Diagnosis and treatment of polycystic ovary syndrome (PCOS): An interview with Richard Legro. *BMC Medicine*, **13**: 64.

Lemmens, S., 1994. 'Plant resources of South-East Asia', *Universitas Indonesia Library*. URL: Pudoc Wageningen, Netherlands (diakses tanggal 11/12/2021).

Li, Z., Alyamani, M., Li, J., Rogacki, K., Abazeed, M., Upadhyay, S.K., dkk., 2016. Redirecting abiraterone metabolism to fine-tune prostate cancer anti-androgen therapy. *Nature*, **533**: 547–551.

Lin, T.-C. dan Hsu, F.-L., 1999. Tanin and Related Compounds from Terminalia catappa and Terminalia parviflora. *Journal of the Chinese Chemical Society*, **46**: 613–618.

Liu, S., Alnammi, M., Ericksen, S.S., Voter, A.F., Ananiev, G.E., Keck, J.L., dkk., 2019. Practical Model Selection for Prospective Virtual Screening. *Journal of Chemical Information and Modeling*, **59**: 282–293.

Macías, F.A., Mejías, F.J., dan Molinillo, J.M., 2019. Recent advances in allelopathy for weed control: from knowledge to applications. *Pest Management Science*, **75**: 2413–2436.

McCartney, C.R. dan Marshall, J.C., 2016. CLINICAL PRACTICE. Polycystic Ovary Syndrome. *The New England Journal of Medicine*, **375**: 54–64.

Mendez, D., Gaulton, A., Bento, A.P., Chambers, J., De Veij, M., Félix, E., dkk., 2019. ChEMBL: towards direct deposition of bioassay data. *Nucleic Acids Research*, **47**: D930–D940.

Meng, X.-Y., Zhang, H.-X., Mezei, M., dan Cui, M., 2011. Molecular Docking: A powerful approach for structure-based drug discovery. *Current computer-aided drug design*, **7**: 146–157.

Messinis, I.E., 2005. Ovulation induction: a mini review. *Human Reproduction (Oxford, England)*, **20**: 2688–2697.

MOE, 2015. Molecular Operating Environment 2015.10.

Nelson, V.L., Legro, R.S., Strauss, J.F., dan McAllister, J.M., 1999. Augmented androgen production is a stable steroidogenic phenotype of propagated theca cells from polycystic ovaries. *Molecular Endocrinology (Baltimore, Md.)*, **13**: 946–957.

Norel, R., Fischer, D., Wolfson, H.J., dan Nussinov, R., 1994. Molecular surface recognition by a computer vision-based technique. *Protein Engineering*, **7**: 39–46.

Norman, R.J., Dewailly, D., Legro, R.S., dan Hickey, T.E., 2007. Polycystic ovary syndrome. *Lancet (London, England)*, **370**: 685–697.

Nunes, R.R., da Fonseca, A.L., Pinto, A.C. de S., Maia, E.H.B., da Silva, A.M., Varotti, F. de P., dkk., 2019. Brazilian malaria molecular targets (BraMMT): selected receptors for virtual high-throughput screening experiments. *Memórias do Instituto Oswaldo Cruz*, **114**: e180465.

Oktarina, A., Abadi, A., dan Bachsin, R., 2014. Faktor-faktor yang Memengaruhi Infertilitas pada Wanita di Klinik Fertilitas Endokrinologi Reproduksi. *Majalah Kedokteran Sriwijaya*, **46**: 295–300.

Oskarsson, A., Spatafora, C., Tringali, C., dan Andersson, Å.O., 2014. Inhibition of CYP17A1 activity by resveratrol, piceatannol, and synthetic resveratrol analogs. *The Prostate*, **74**: 839–851.

Palomba, S., de Wilde, M.A., Falbo, A., Koster, M.P.H., La Sala, G.B., dan Fauser, B.C.J.M., 2015. Pregnancy complications in women with polycystic ovary syndrome. *Human Reproduction Update*, **21**: 575–592.

Pándy-Szekeres, G., Esguerra, M., Hauser, A.S., Caroli, J., Munk, C., Pilger, S., dkk., 2021. The G protein database, GproteinDb. *Nucleic Acids Research*, gkab852.

Pastor, C.L., Griffin-Korf, M.L., Aloi, J.A., Evans, W.S., dan Marshall, J.C., 1998. Polycystic ovary syndrome: evidence for reduced sensitivity of the gonadotropin-releasing hormone pulse generator to inhibition by estradiol and progesterone. *The Journal of Clinical Endocrinology and Metabolism*, **83**: 582–590.

Pauly, G., 2001. 'Cosmetic, dermatological and pharmaceutical use of an extract of terminalia catappa', [*patent*] US20010002265A1.

Peach, M.L. dan Nicklaus, M.C., 2009. Combining docking with pharmacophore filtering for improved virtual screening. *Journal of Cheminformatics*, **1**: 6.

Petrunak, E.M., Rogers, S.A., Aubé, J., dan Scott, E.E., 2017. Structural and Functional Evaluation of Clinically Relevant Inhibitors of Steroidogenic Cytochrome P450 17A1. *Drug Metabolism and Disposition*, **45**: 635–645.

Ramírez, D. dan Caballero, J., 2018. Is It Reliable to Take the Molecular Docking Top Scoring Position as the Best Solution without Considering Available Structural Data? *Molecules : A Journal of Synthetic Chemistry and Natural Product Chemistry*, **23**: 1038.

Rarey, M., Kramer, B., Lengauer, T., dan Klebe, G., 1996. A fast flexible docking method using an incremental construction algorithm. *Journal of Molecular Biology*, **261**: 470–489.

Rester, U., 2008. From virtuality to reality - Virtual screening in lead discovery and lead optimization: a medicinal chemistry perspective. *Current Opinion in Drug Discovery & Development*, **11**: 559–568.

Singh, N., Singh Rao, A., Nandal, A., Kumar, S., Yadav, S., Ganie, S., dkk., 2020. Phytochemical and pharmacological review of Cinnamomum verum J.

Presl-a versatile spice used in food and nutrition. *Food Chemistry*, **338**: 127773.

Siriwardene, S.A., Karunathilaka, L.P.A., Kodituwakku, N.D., dan Karunarathne, Y. a. U.D., 2010. Clinical efficacy of Ayurveda treatment regimen on Subfertility with Poly Cystic Ovarian Syndrome (PCOS). *Ayu*, **31**: 24–27.

Sterling, T. dan Irwin, J.J., 2015. ZINC 15 – Ligand Discovery for Everyone. *Journal of Chemical Information and Modeling*, **55**: 2324–2337.

Sudarmanto, B.S.A., Yuswanto, A., Susidarti, R.A., dan Noegrohati, S., 2017. Molecular Modeling of Human 3β-Hydroxysteroid Dehydrogenase Type 2: Combined Homology Modeling, Docking and QSAR Approach. *JURNAL ILMU KEFARMASIAN INDONESIA*, **15**: 7–16.

Sweetnam, P.M., Price, C.H., dan Ferkany, J.W., 1995. *Burger's Medicinal Chemistry and Drug Discovery*. John Wiley & Sons, New York.

Tanaka, T., Nonaka, G.-I., dan Nishioka, I., 1986. Tanins and related compounds. XLII. Isolation and characterization of four new hydrolyzable tanins, terflavins A and B, tergallagin and tercatain from the leaves of Terminalia catappa L. *Chemical and Pharmaceutical Bulletin*, **34**: 1039–1049.

Tang, T., Lord, J.M., Norman, R.J., Yasmin, E., dan Balen, A.H., 2012. Insulin-sensitising drugs (metformin, rosiglitazone, pioglitazone, D-chiro-inositol) for women with polycystic ovary syndrome, oligo amenorrhoea and subfertility. *The Cochrane Database of Systematic Reviews*, CD003053.

Usha, S. dan Selvaraj, S., 2016. Prediction of kinase-inhibitor binding affinity using energetic parameters. *Bioinformation*, **12**: 172–181.

Wal, A., Wal, P., Saraswat, N., dan Wadhwa, S., 2021. A Detailed Review on Herbal Treatments for Treatment of PCOS- Polycystic ovary syndrome (PCOS). *Current Nutraceuticals*, **2**: 192–202.

Yoshimoto, F.K. dan Auchus, R.J., 2015. The diverse chemistry of cytochrome P450 17A1 (P450c17, CYP17A1). *The Journal of steroid biochemistry and molecular biology*, **151**: 52–65.

Zhang, C., Fan, L., Fan, S., Wang, J., Luo, T., Tang, Y., dkk., 2019. Cinnamomum cassia Presl: A Review of Its Traditional Uses, Phytochemistry, Pharmacology and Toxicology. *Molecules*, **24**: 3473.

Zhang, X.-R., Kaunda, J.S., Zhu, H.-T., Wang, D., Yang, C.-R., dan Zhang, Y.-J., 2019. The Genus Terminalia (Combretaceae): An Ethnopharmacological, Phytochemical and Pharmacological Review. *Natural Products and Bioprospecting*, **9**: 357–392.